SOLID STATE STUDIES:

TRANSITION IONS IN ZINC OXIDE

VOLUME II

A thesis presented for the
degree of Doctor of Philosophy in Physics
in the University of Canterbury,
Christchurch, New Zealand.

by

R S Anderson

R. S. Anderson

1967.

TABLE OF FIGURES, APPENDICES, AND PROGRAM LISTINGS

FIGURES

APPENDICES

PROGRAM LISTINGS

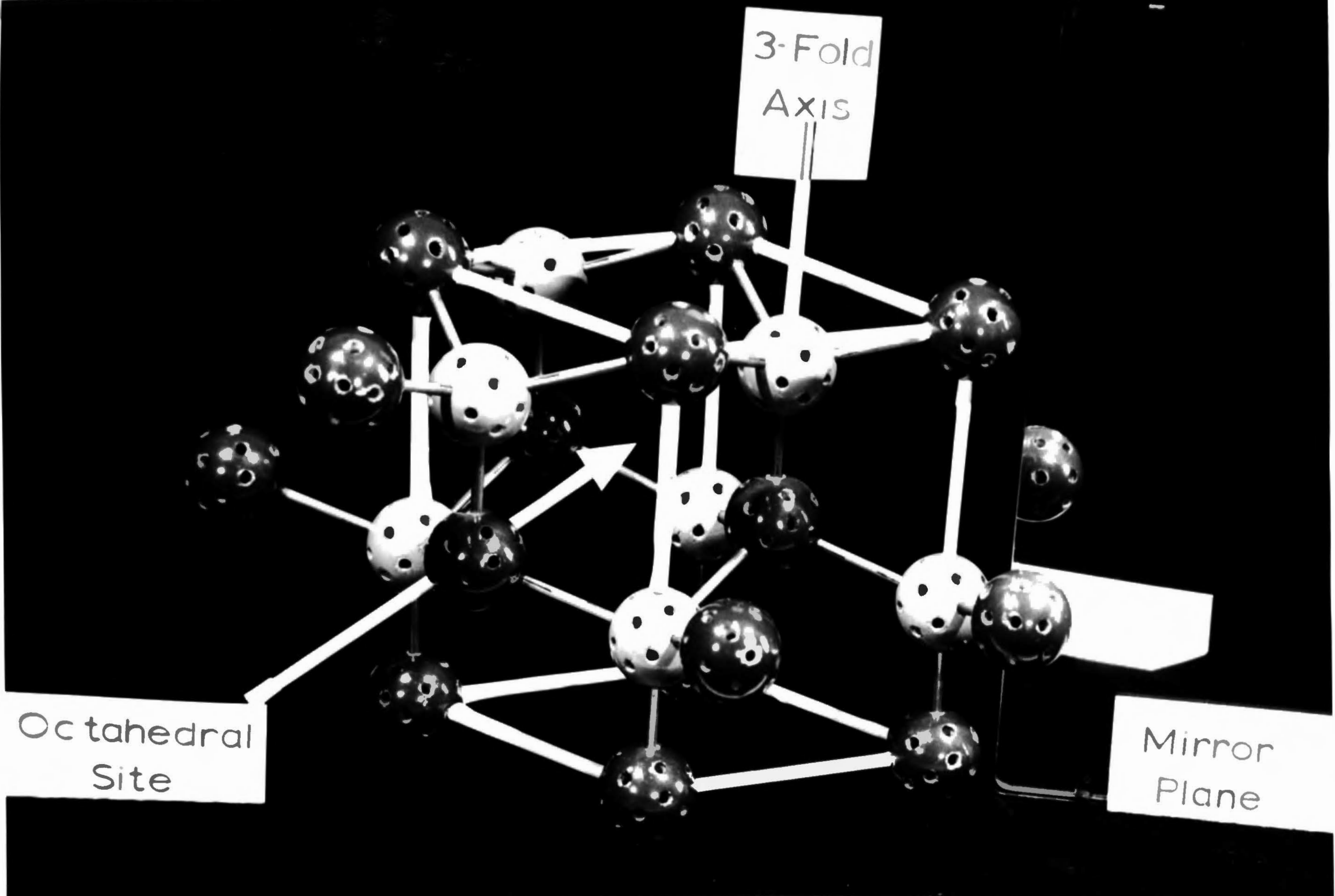
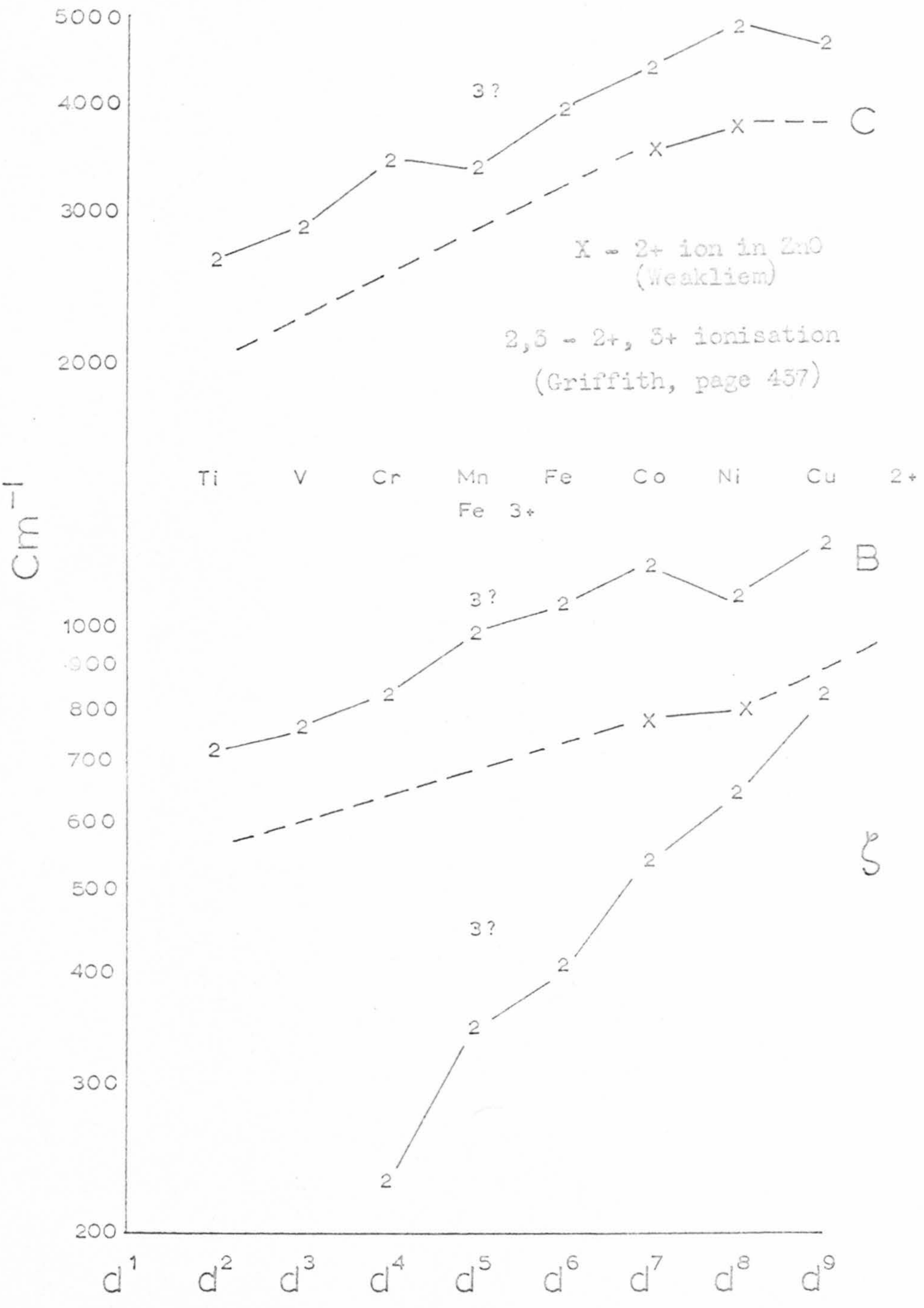


Figure 1-1 The ZnO Wurtzite Structure

Figure 1-2 Free Ion Parameters for the First Transition Series



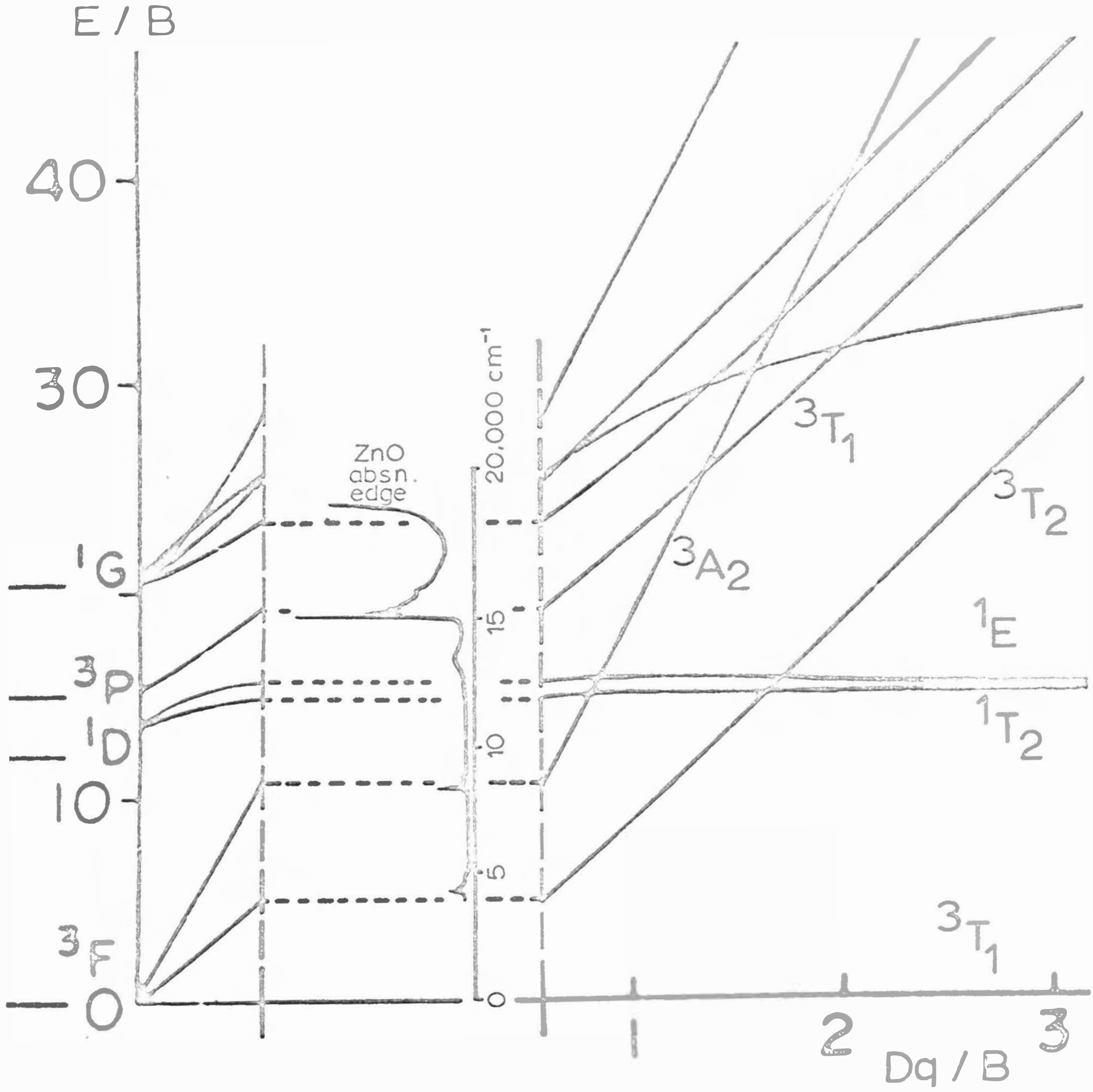
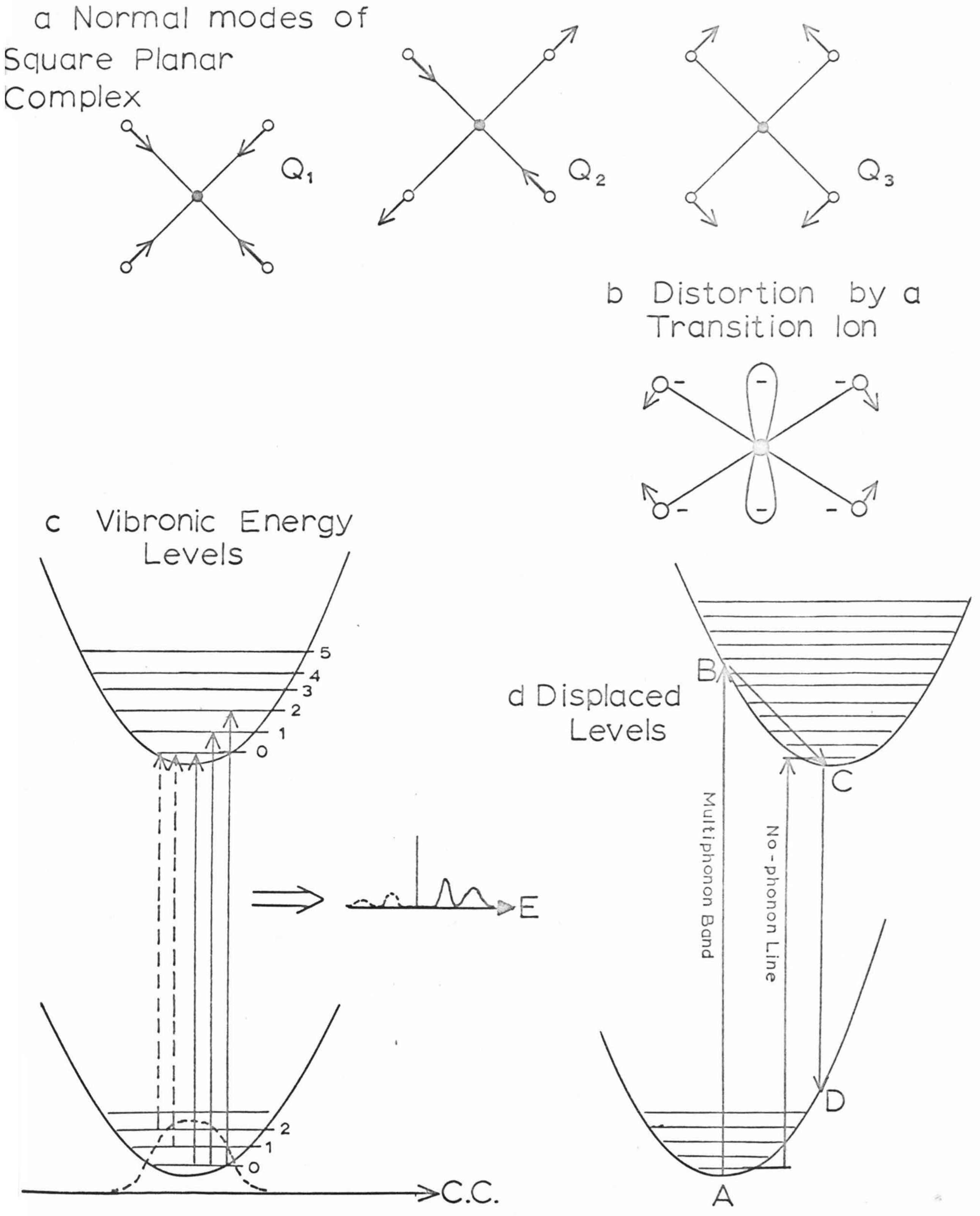


Figure 1-3 Tanabe- Sugano Fit for Ni^{++} - ZnO

Figure 1-4 Electron-Vibration Interaction



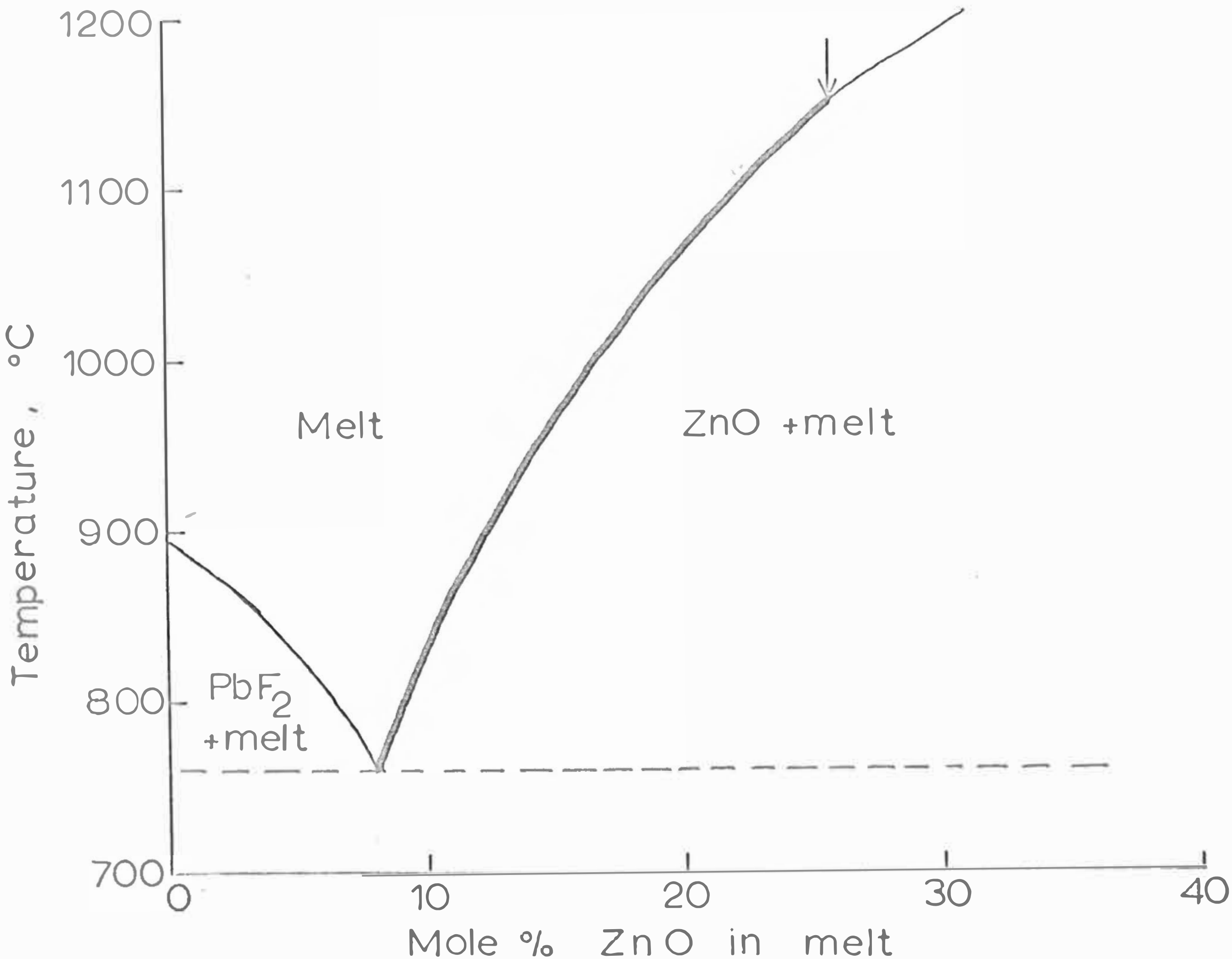


Figure 2-1 PbF_2 / ZnO Phase Diagram

Figure 2-2 Conversion of On/Off to Proportional Control

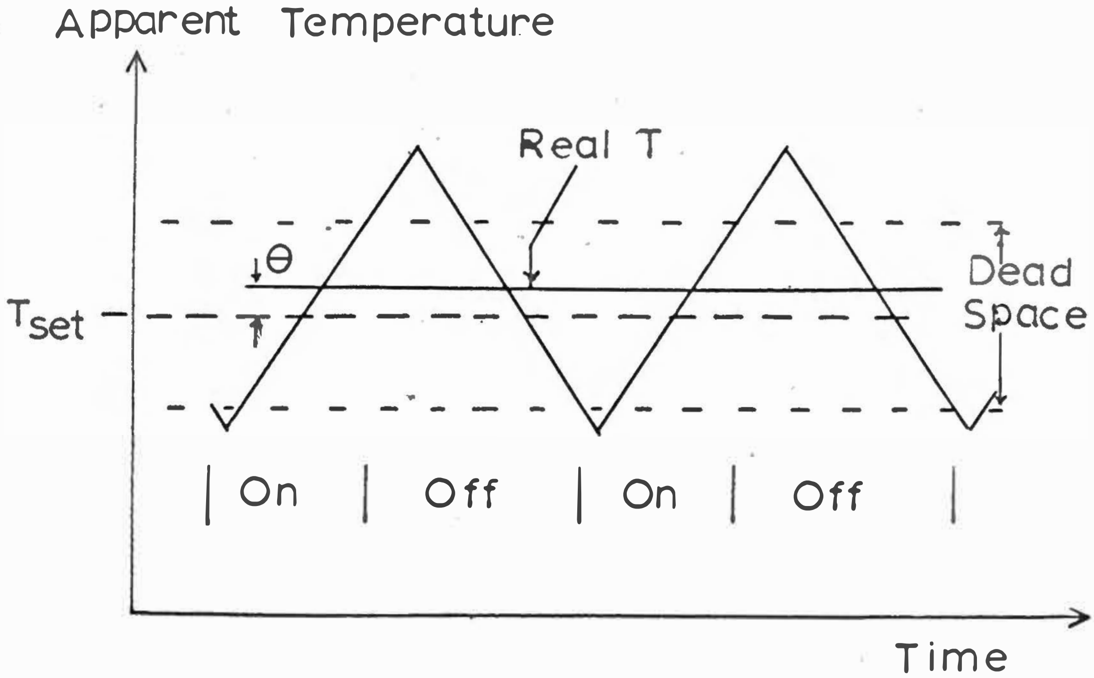


Figure 2-3 Thermocouple Break Protection Circuit

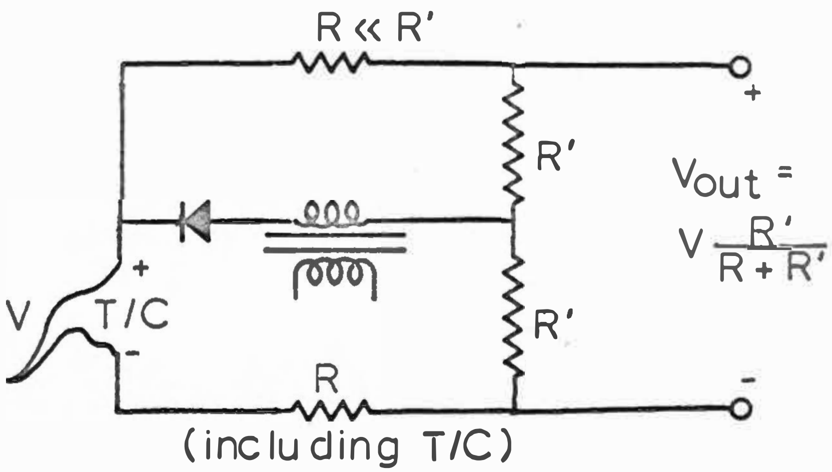


Figure 2-4 Voltage Production Circuit

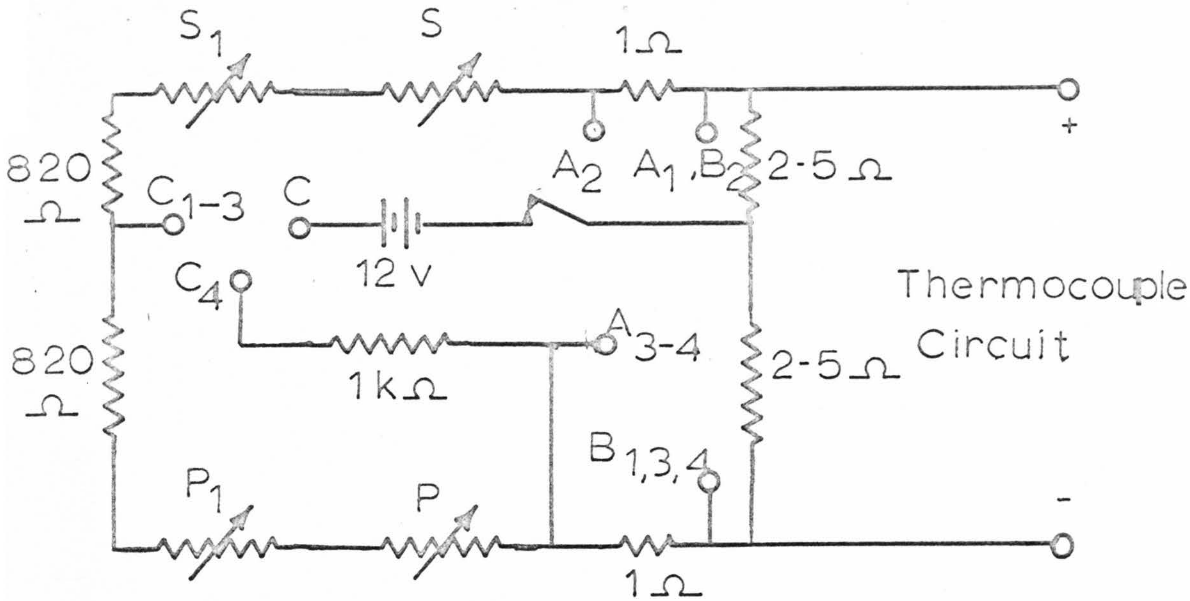
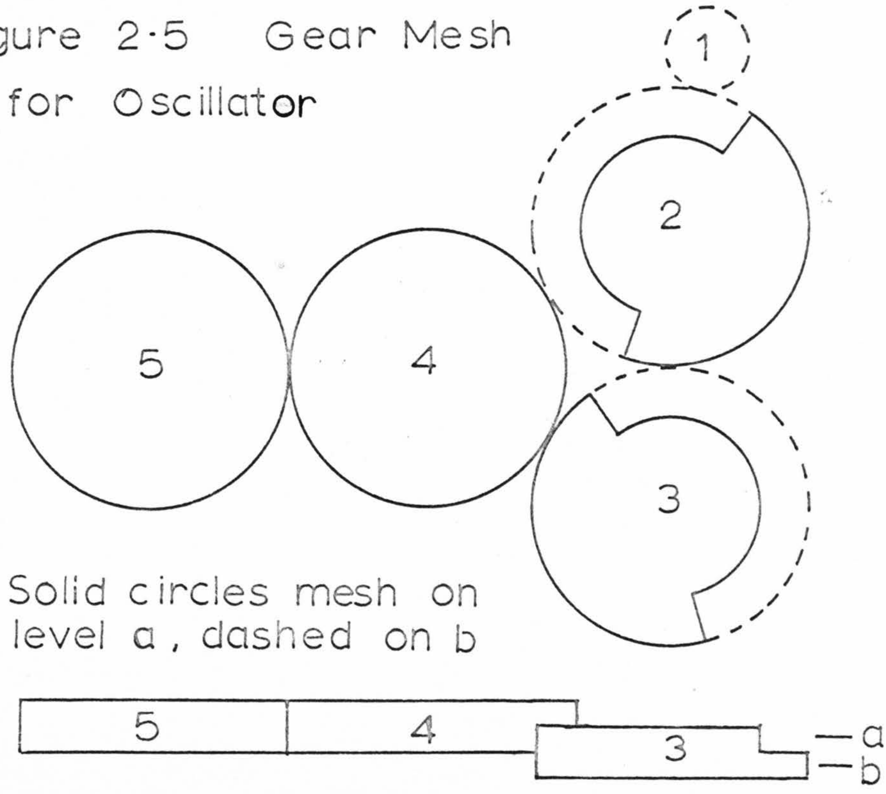


Figure 2-5 Gear Mesh for Oscillator



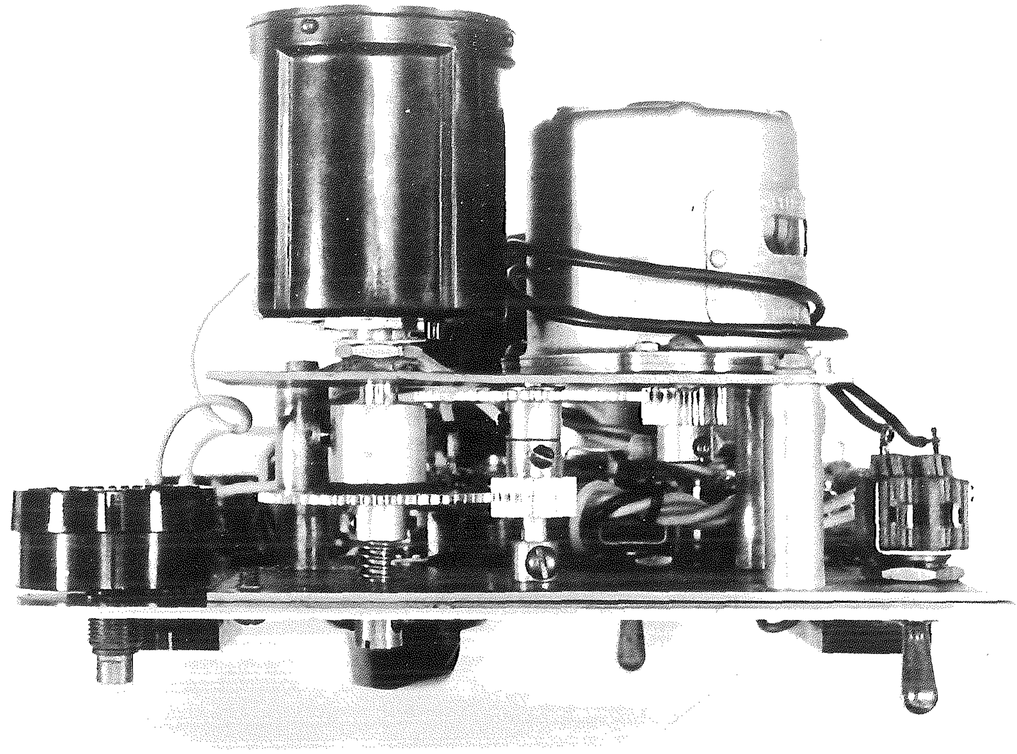
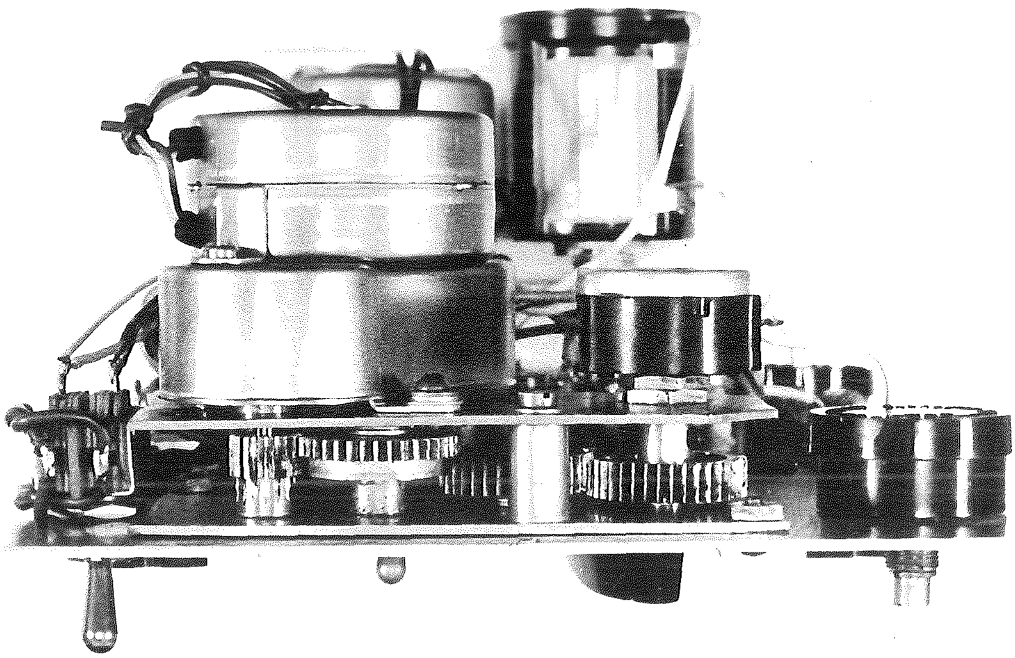


Figure 2·6 Sweep drive

Figure 2·7 Oscillatory drive



Oscillating set point control

Figure 2-8 Panel

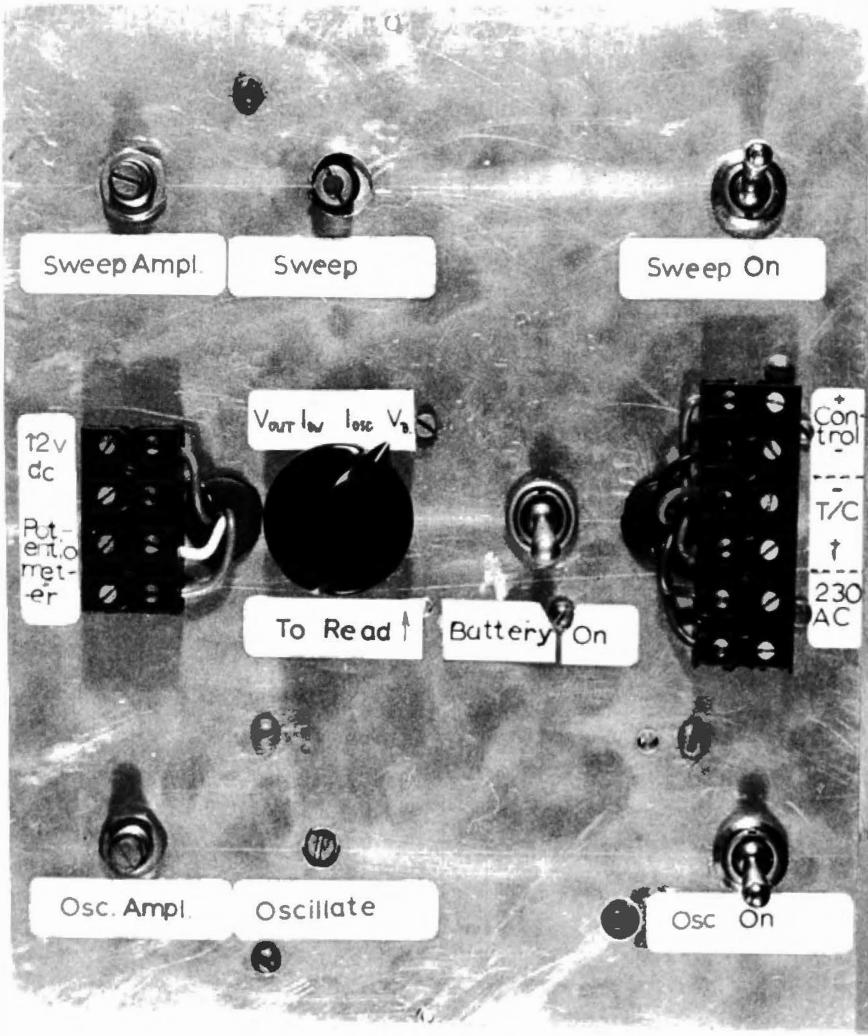
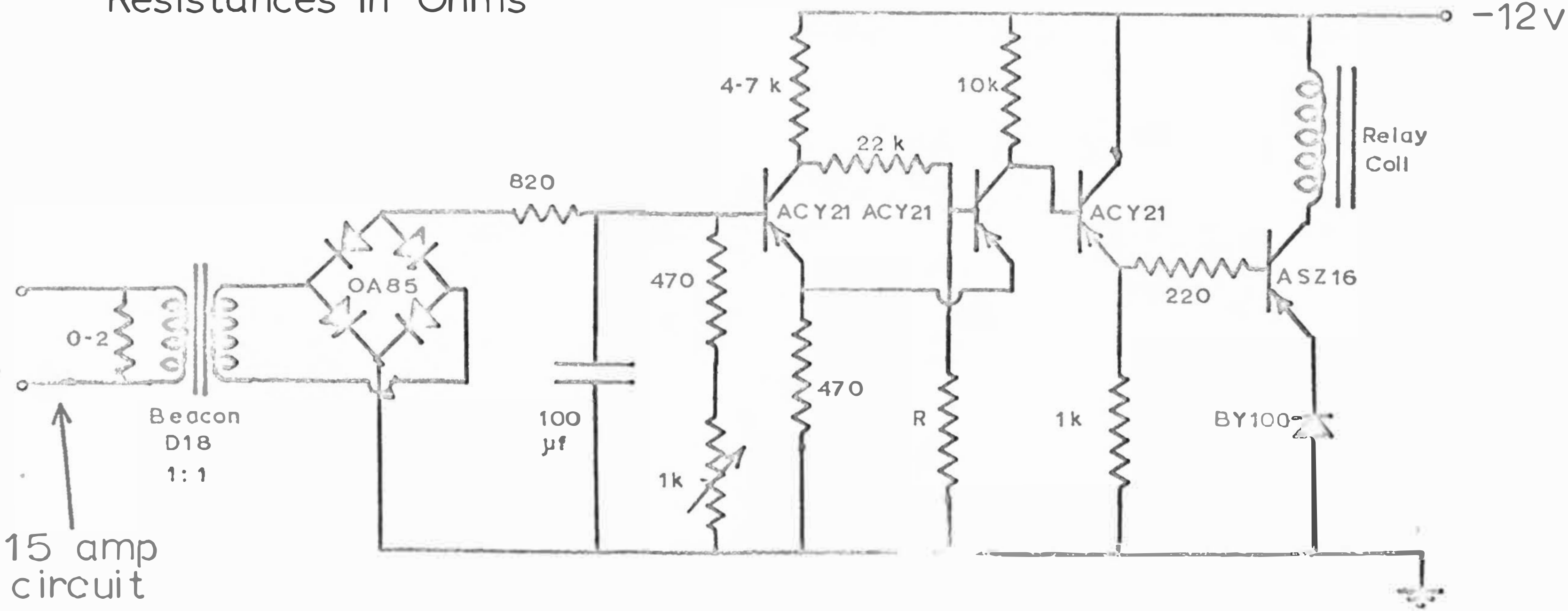


Figure 2-9 Rear

Figure 2-10 Schmitt Trigger

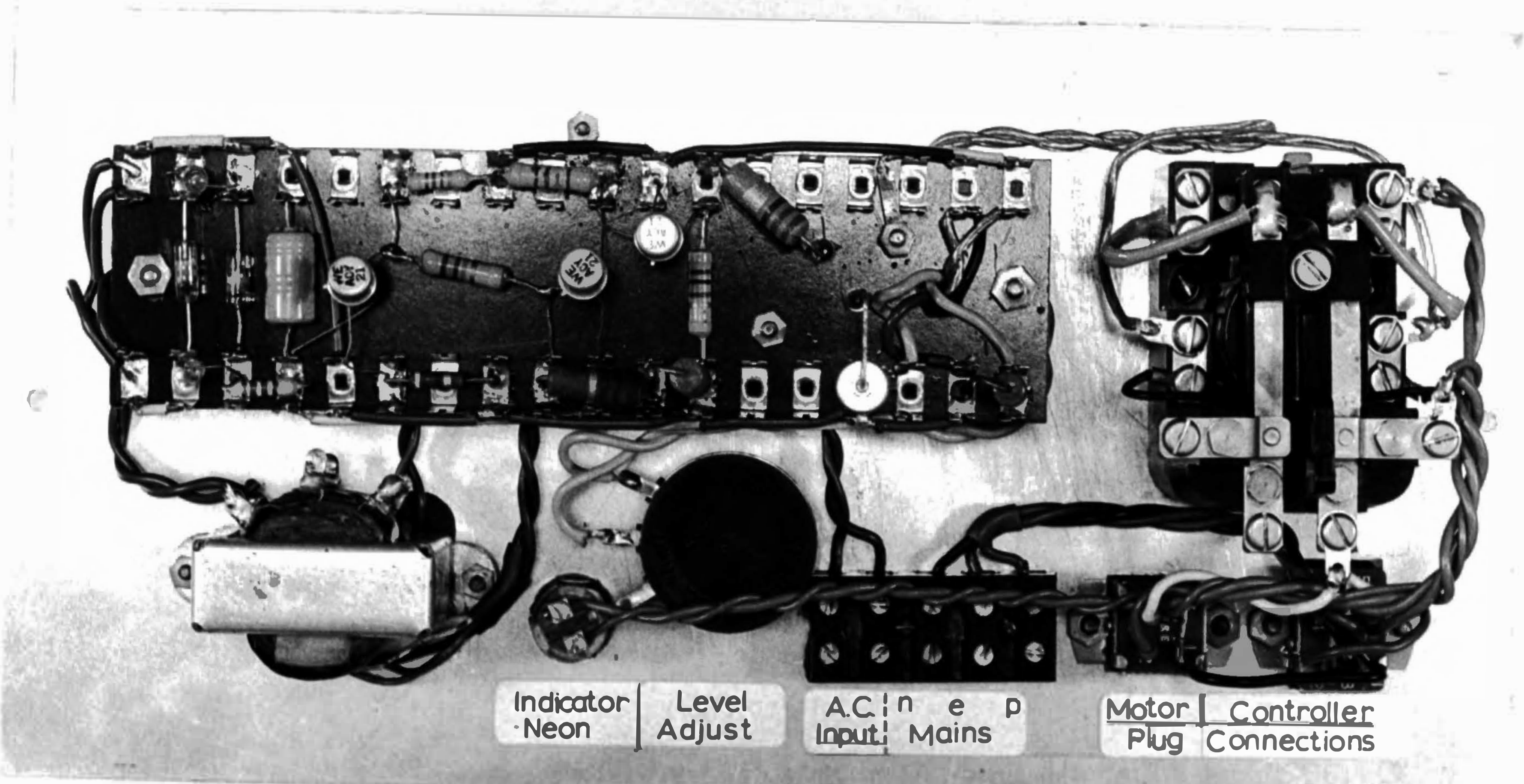
Resistances in Ohms



R for best performance 2420

Relay - Arrow 28308U with 12v coil

Figure 2-11 Schmitt Trigger



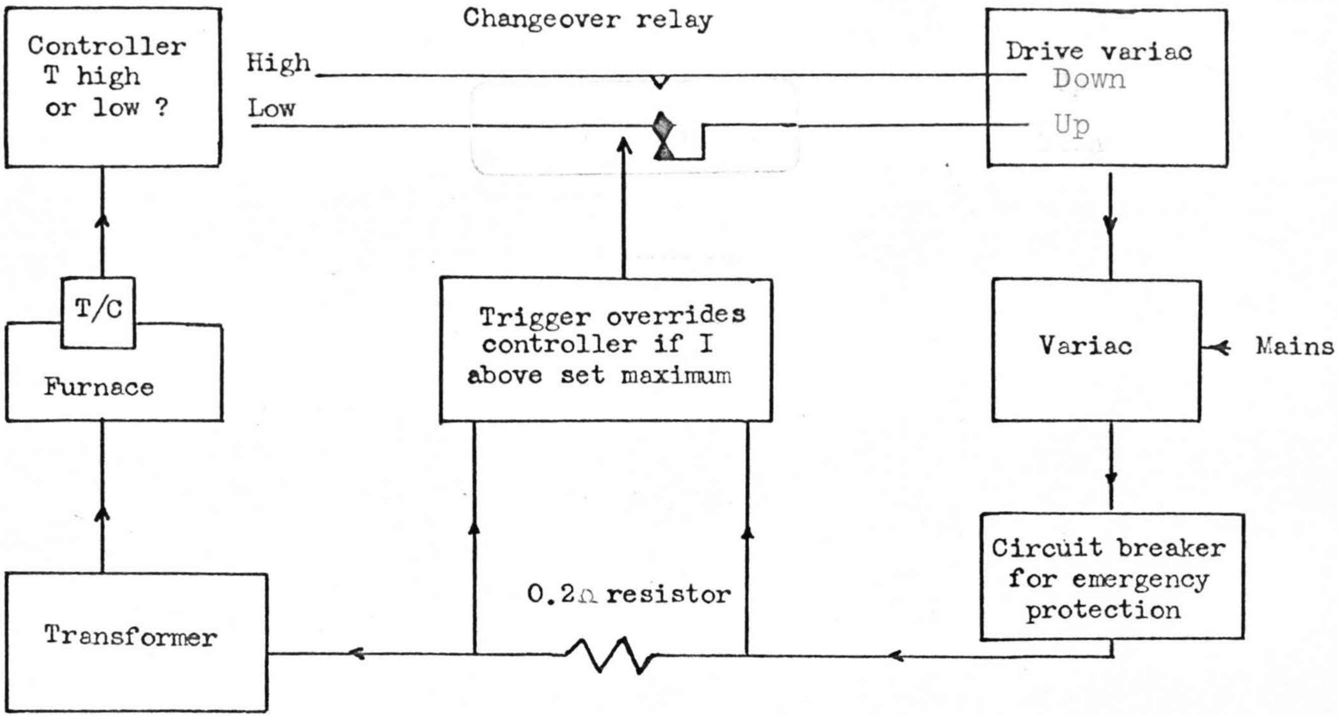


Figure 2.12 Furnace Controller Logic

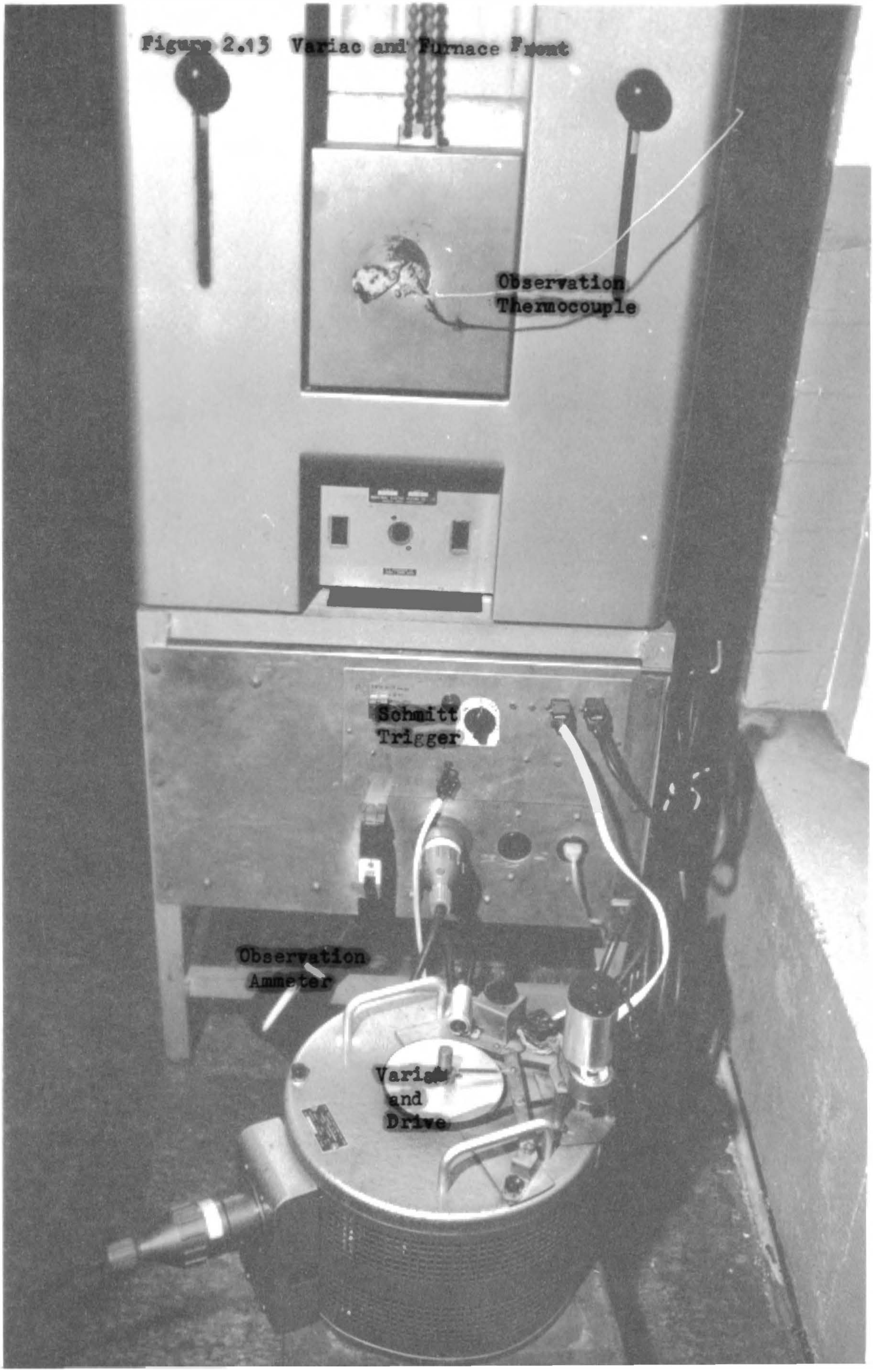
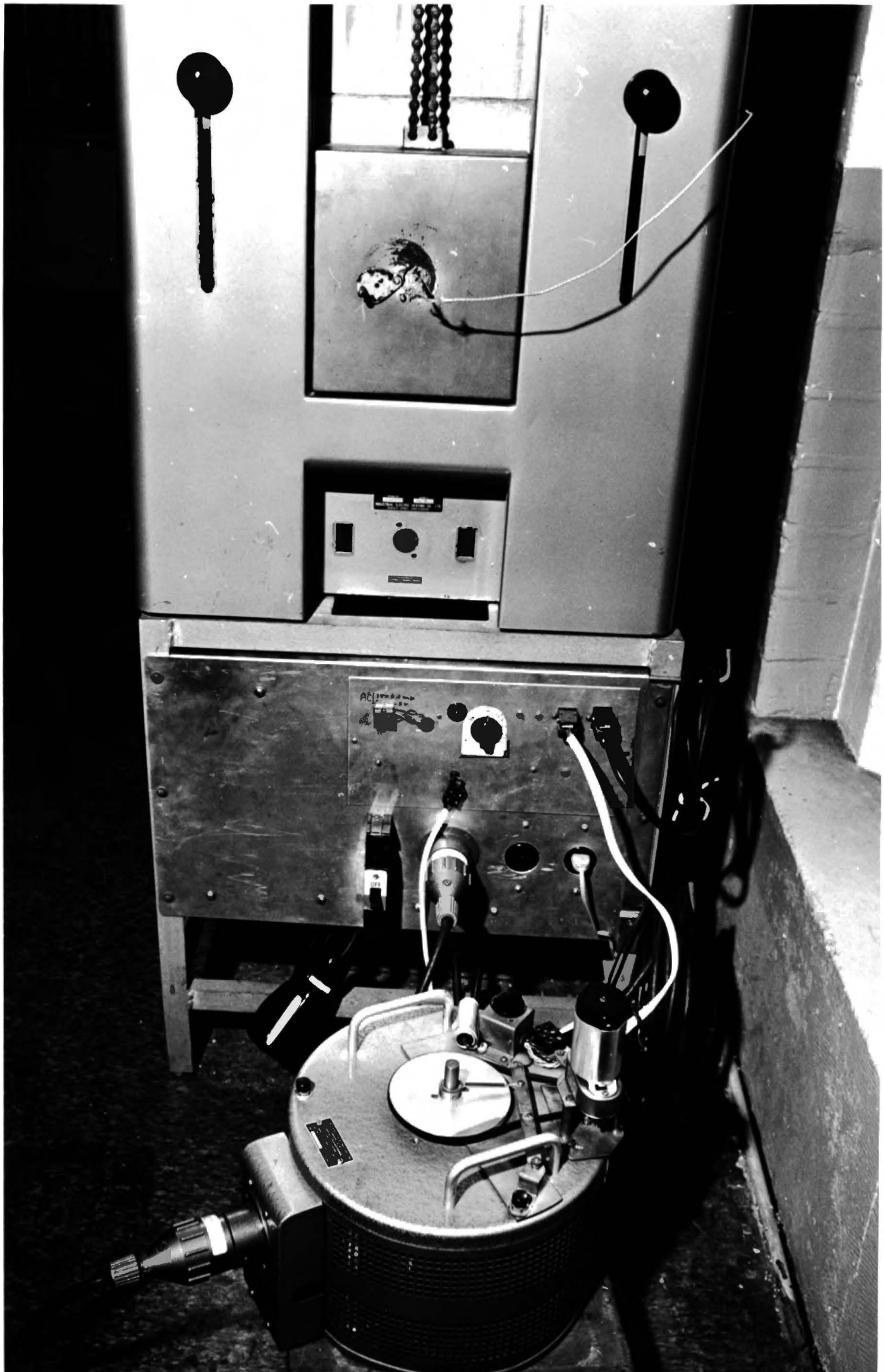


Figure 2.13 Variac and Furnace Front



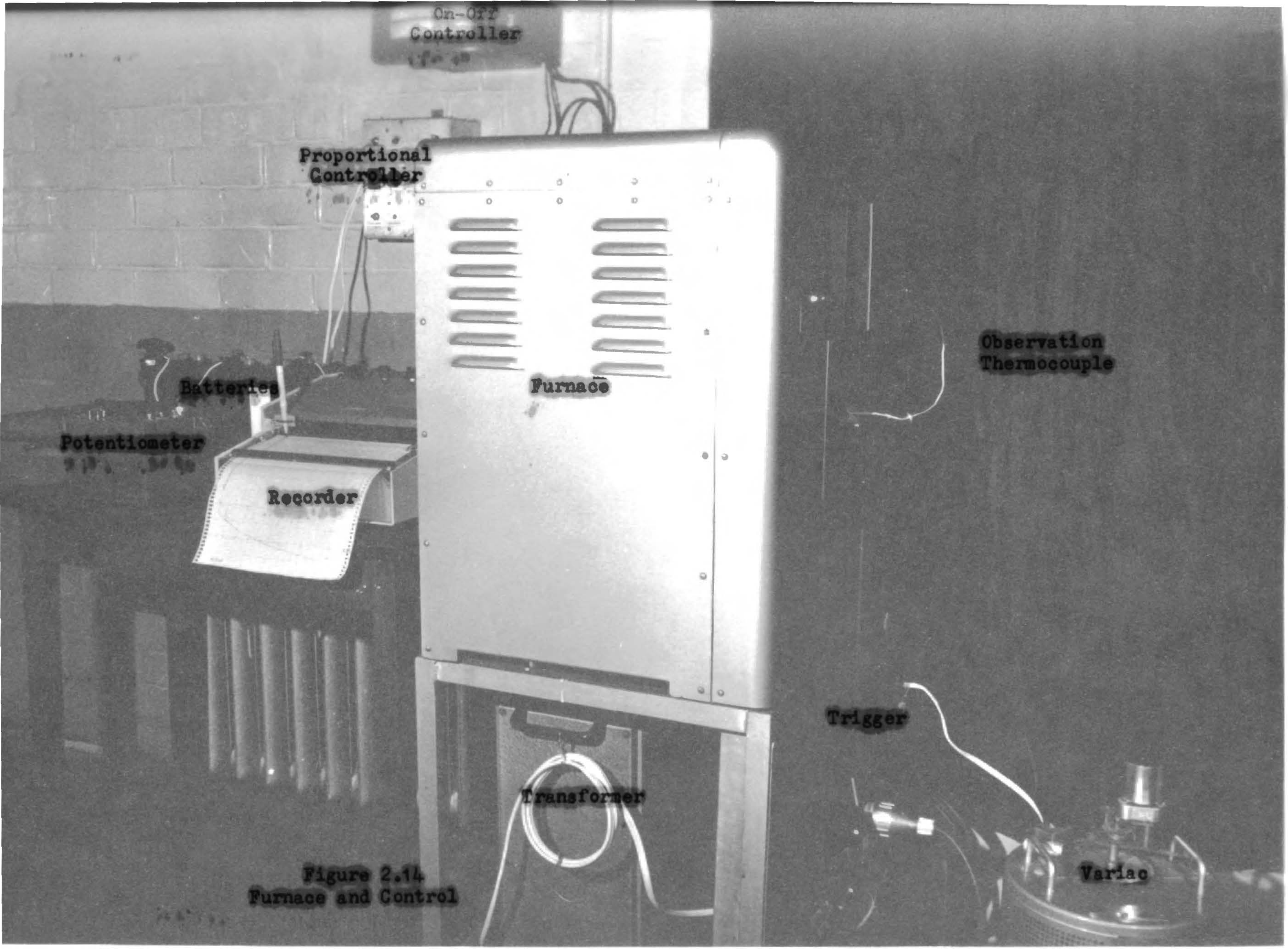
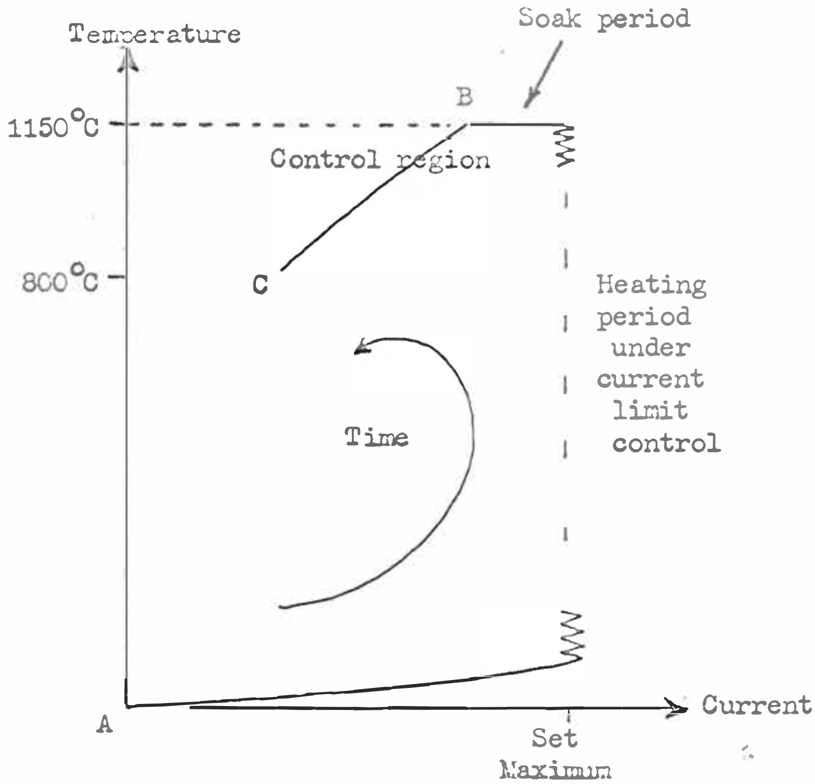


Figure 2.14
Furnace and Control

Figure 2.15

<u>Temperature / Current Plot of</u>

<u>Furnace Operation</u>



<u>OPERATOR CONTROL</u>

A Turn on all but sweep motor

B Start sweep motor after sufficient soak period

C Turn complete system off when temperature low enough

At A, the variac should be set to a low voltage before switching on, so that the starting current is not too large.

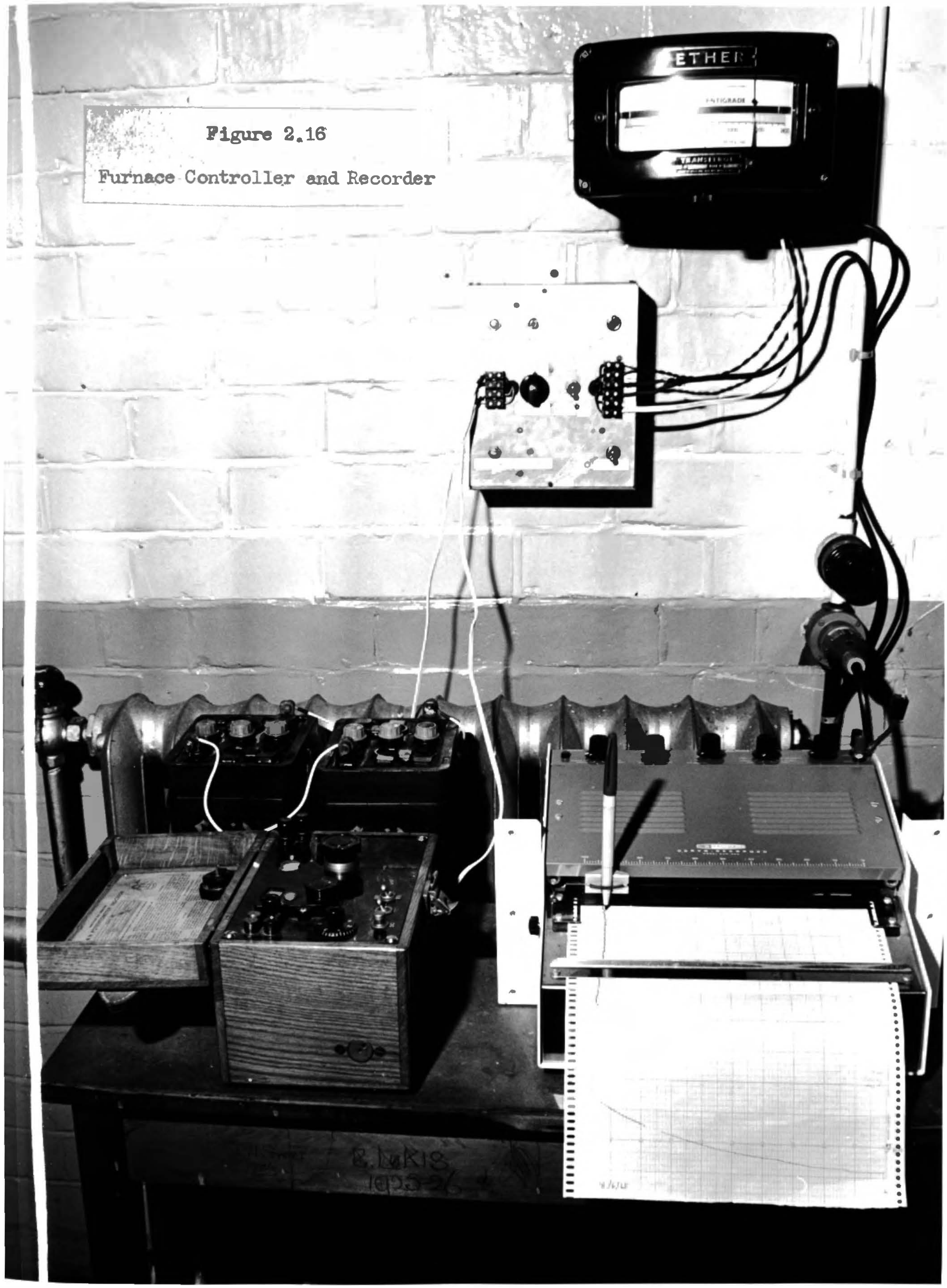


Figure 2.16

Furnace Controller and Recorder

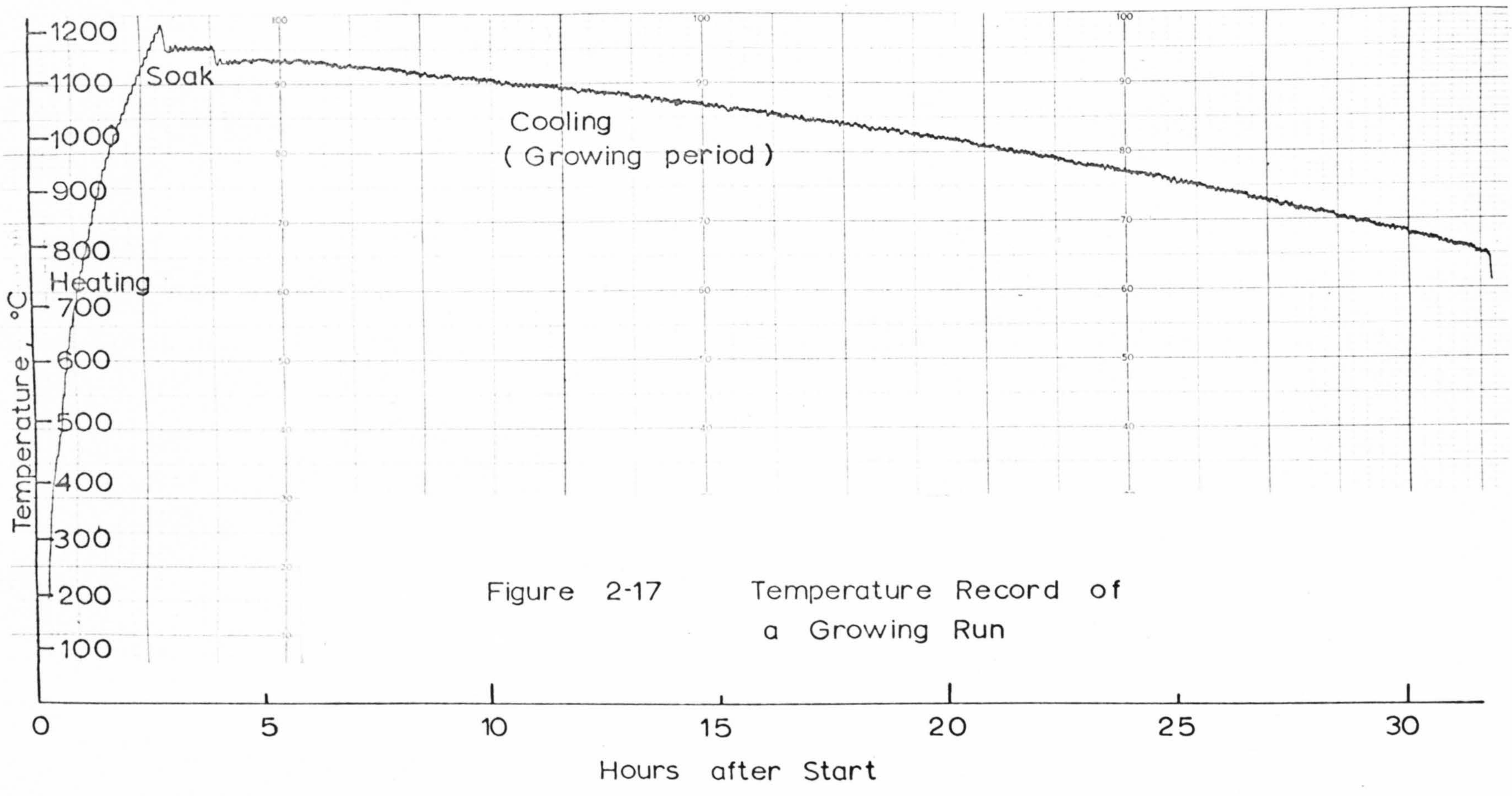


Figure 2-17 Temperature Record of a Growing Run

Figure 2·18 Crucibles in brick
Scale in inches

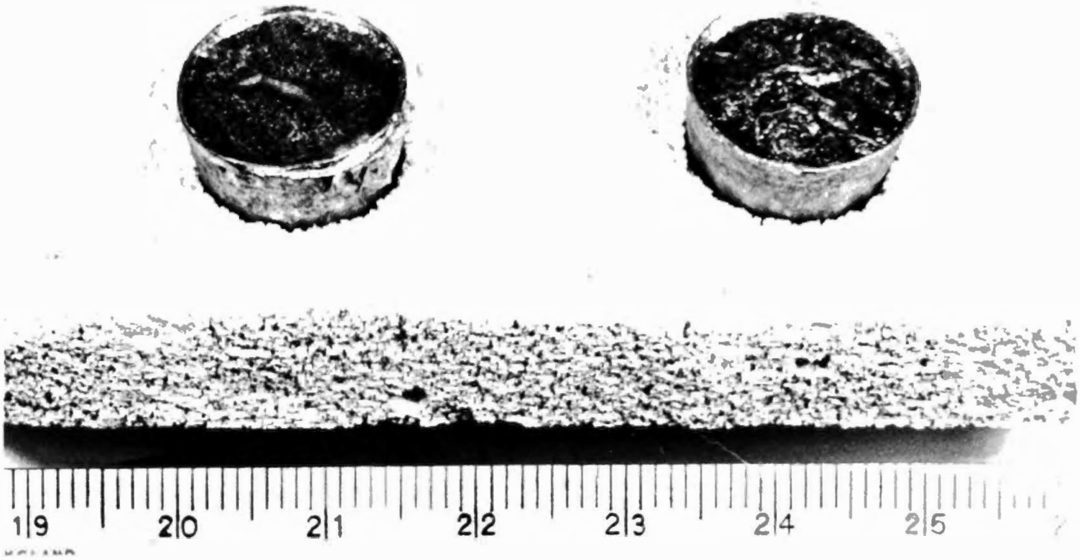
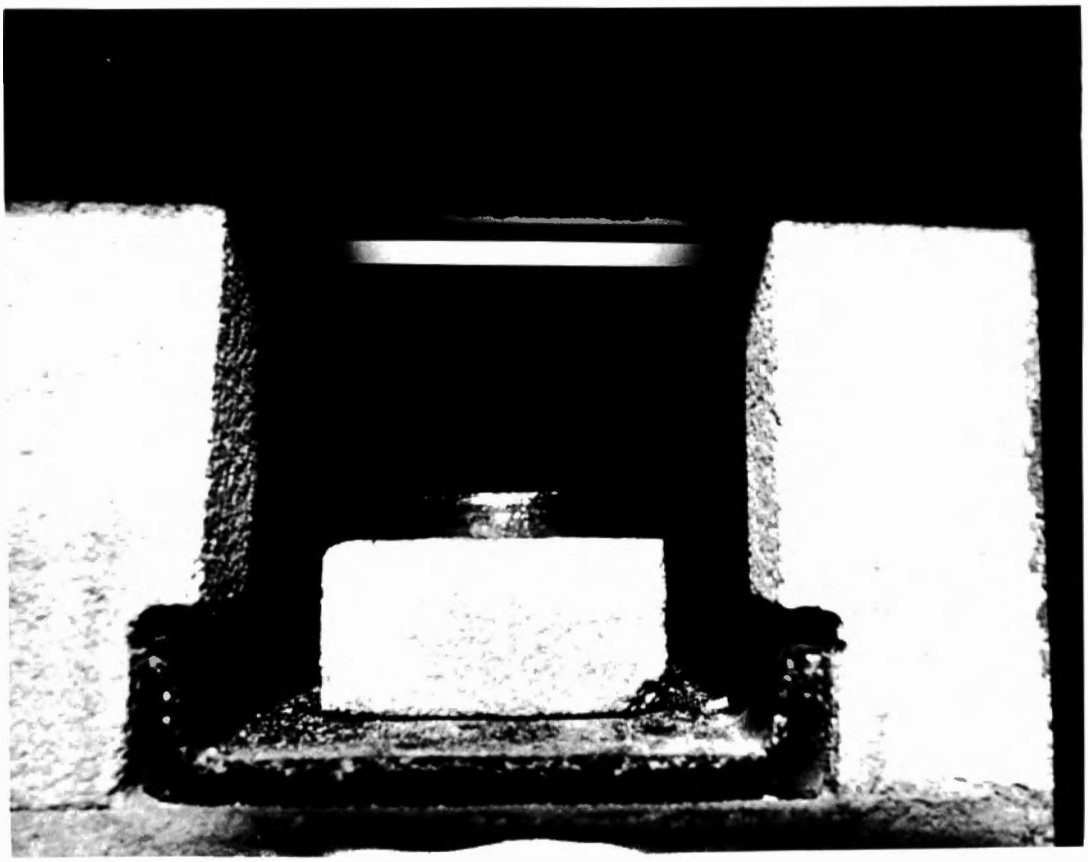


Figure 2·19 Crucibles in furnace



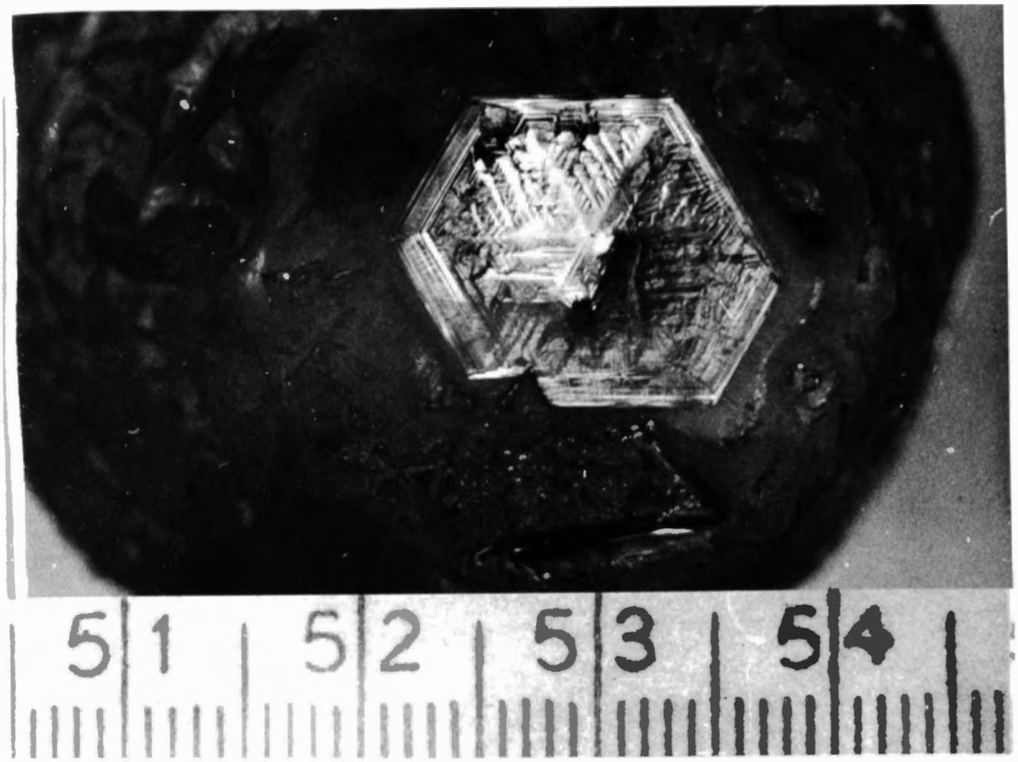


Figure 2-20
Ni^{++}-ZnO
Sample 6

Scale in cm

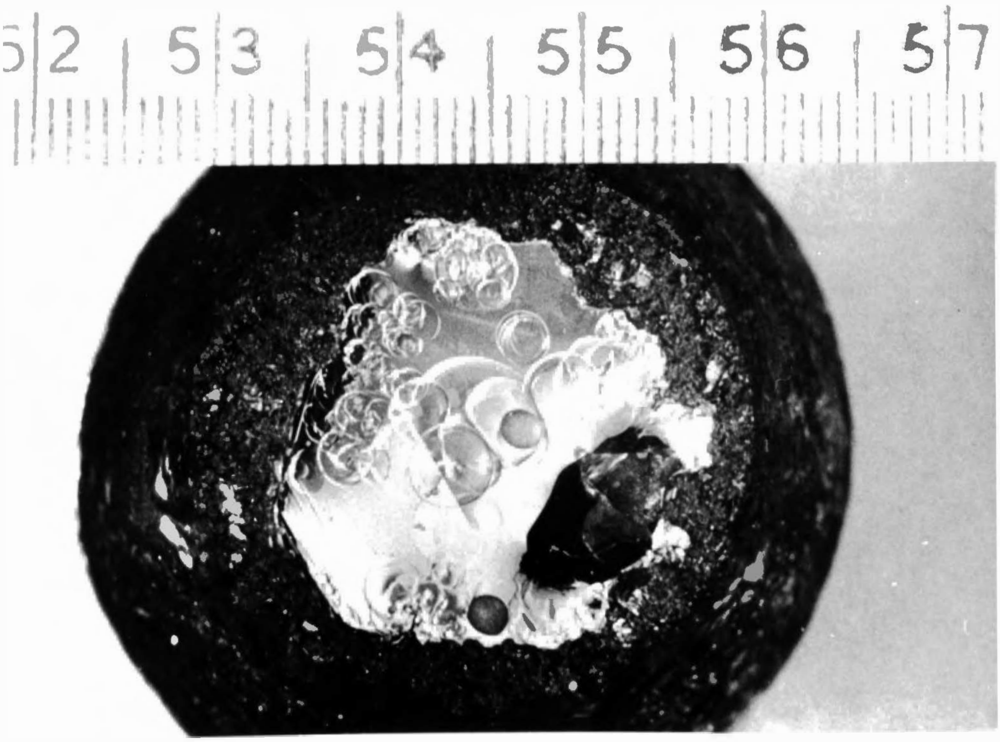


Figure 2-21
Co^{++}-ZnO
Sample 7

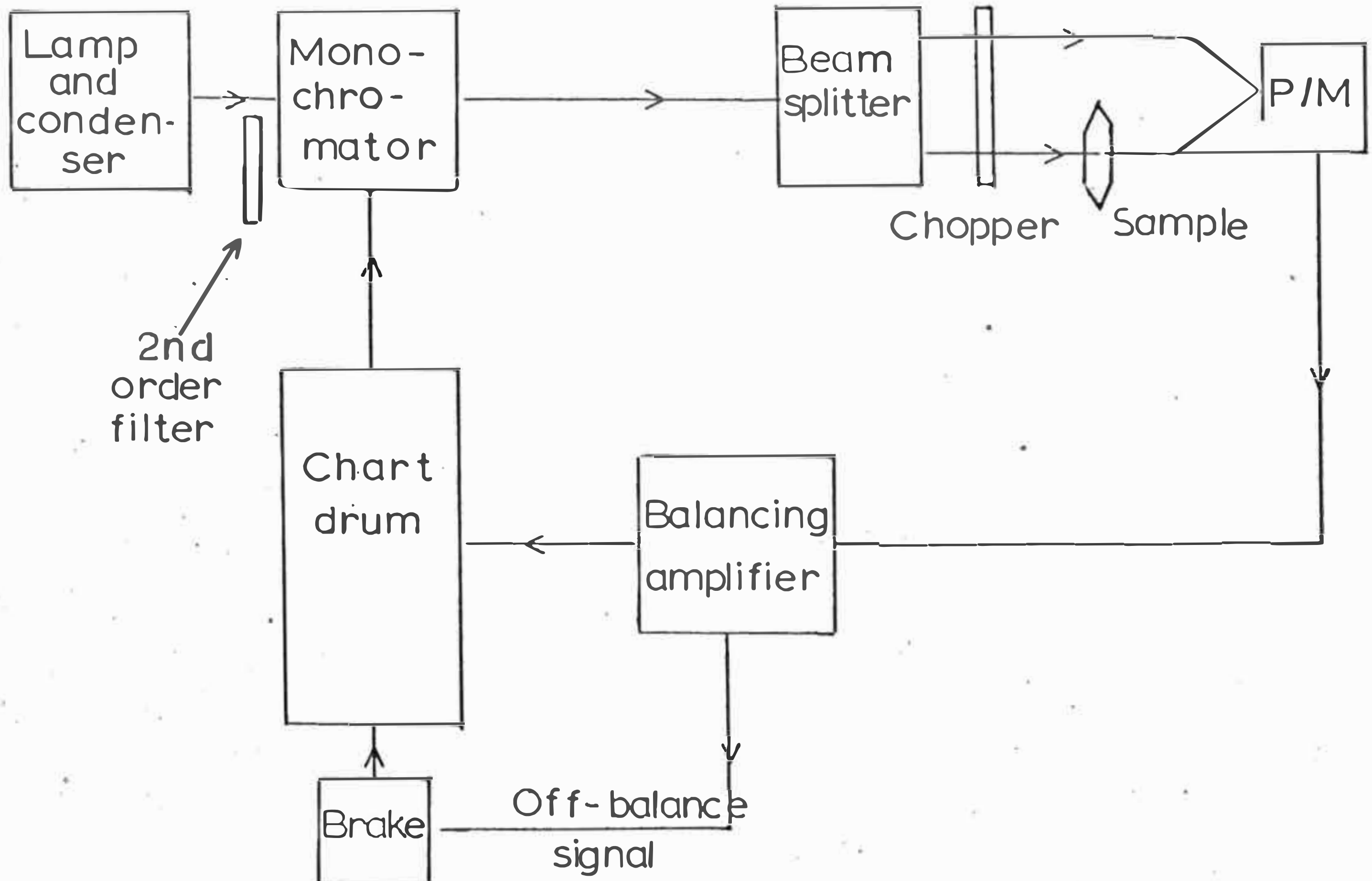


Figure 3-1 Bausch and Lomb Schematics

Figure 3-2

Bausch and Lomb
Sample focus

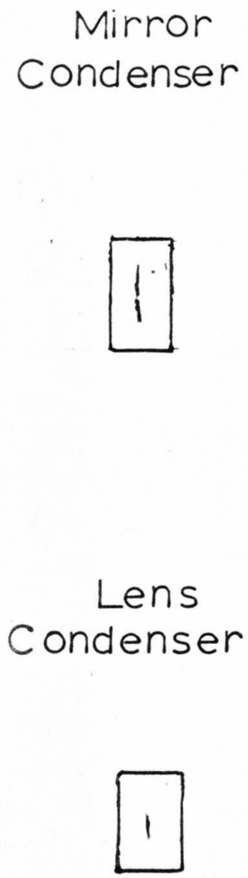
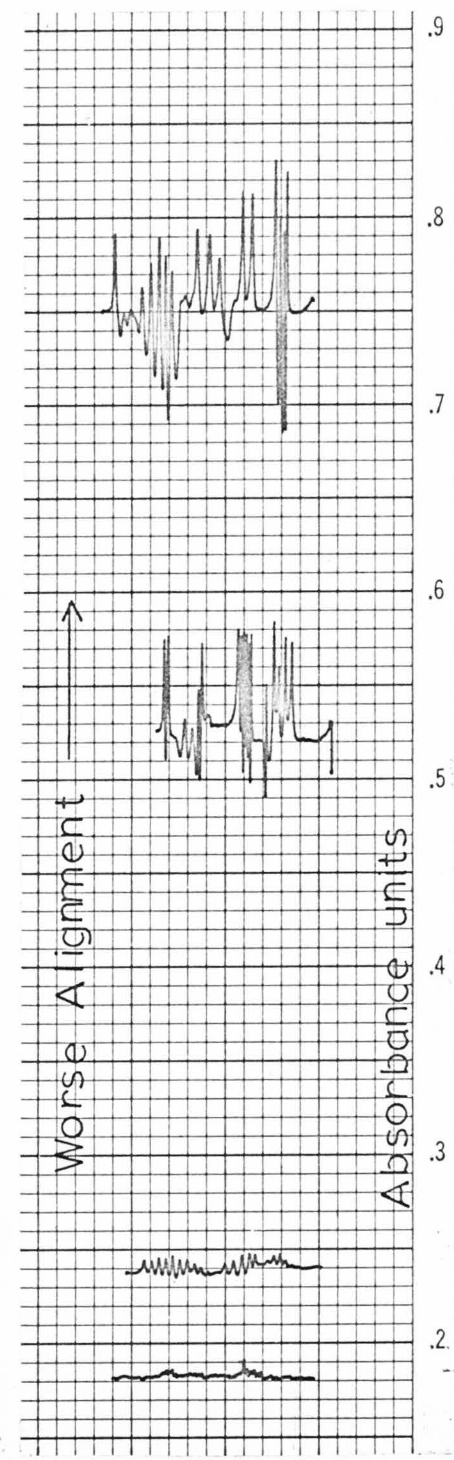


Figure 3-3

Vibration effects



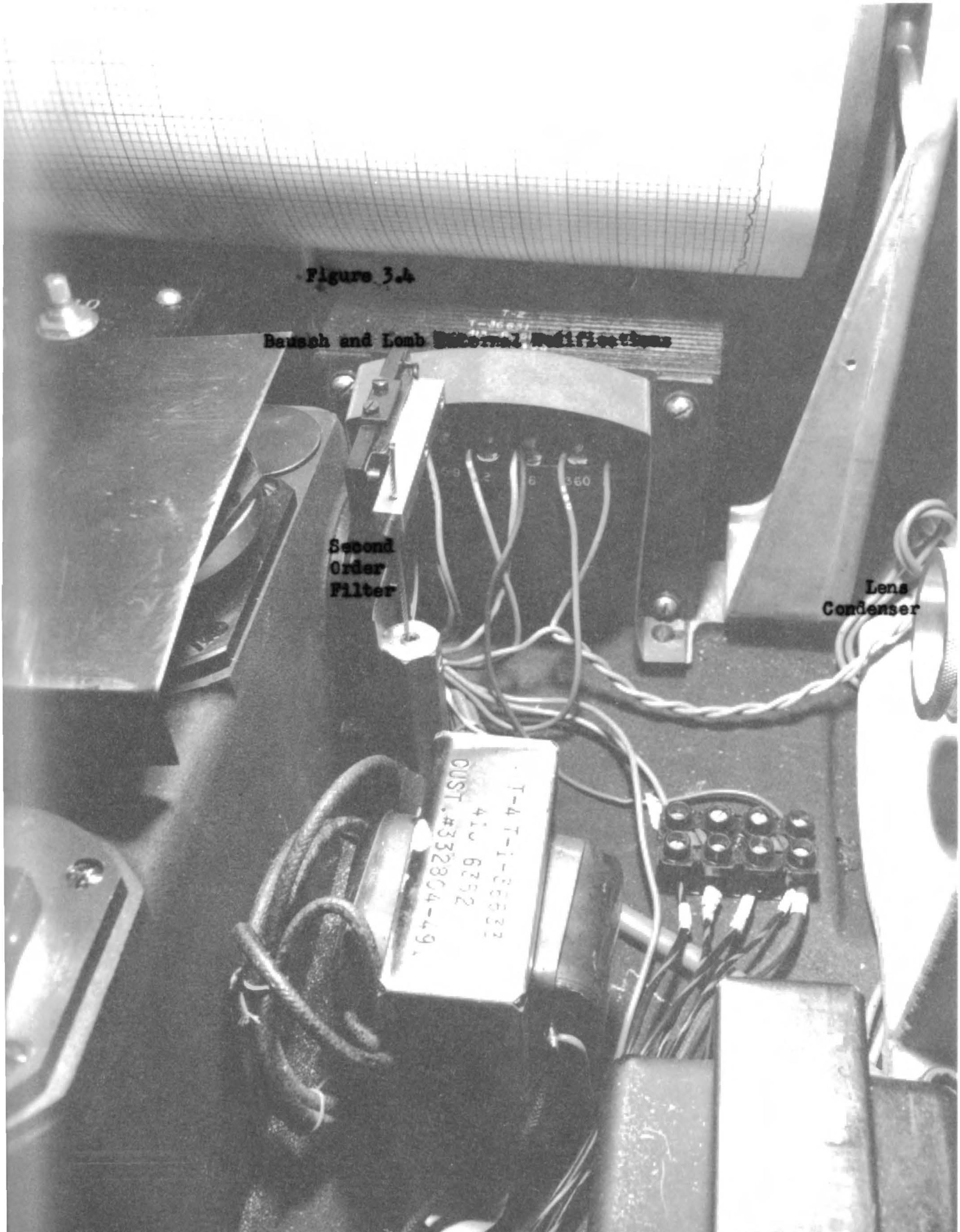


Figure 3.4
Bausch and Lomb [illegible] Modifications
Second
Order
Filter
Lens
Condenser

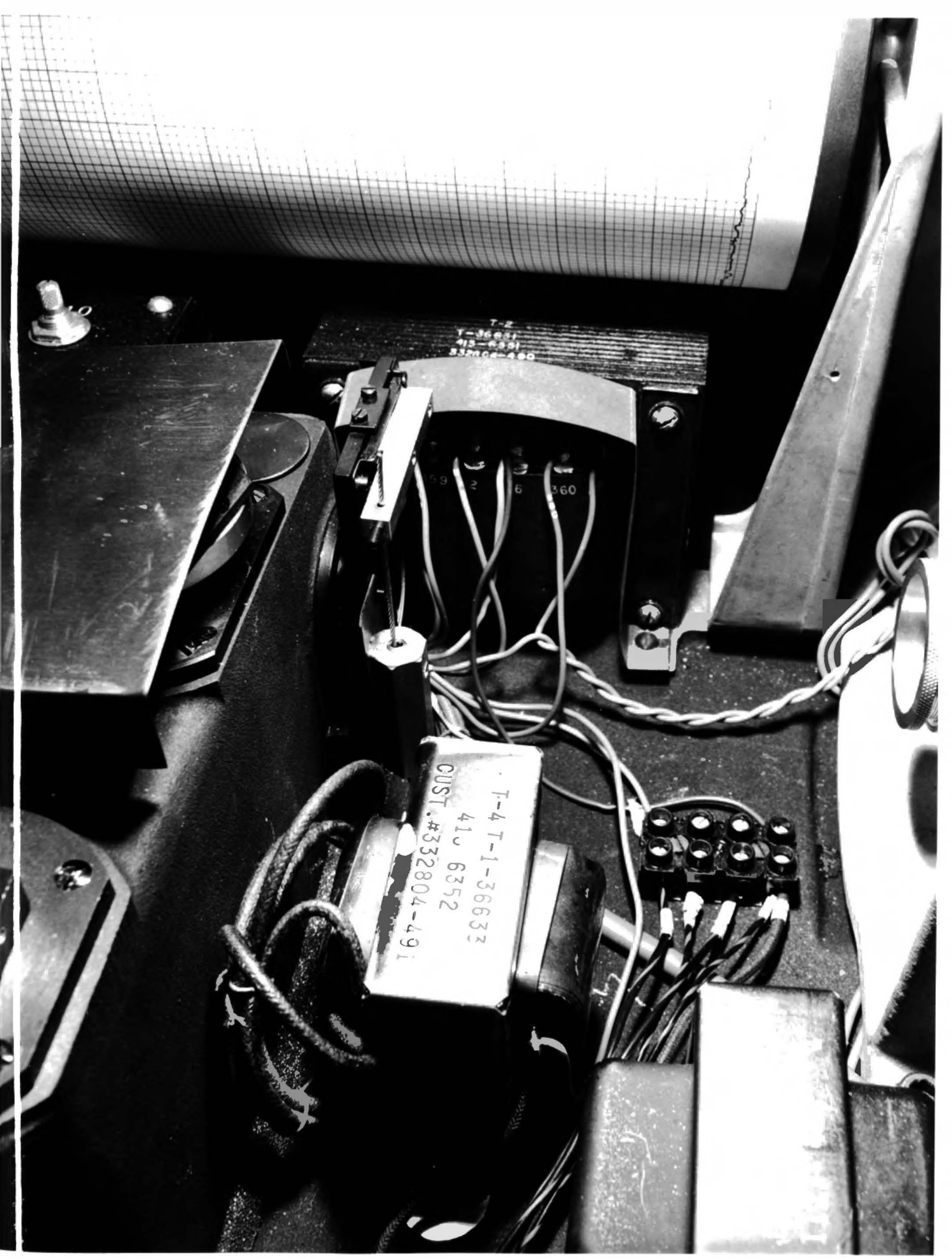

T-2
360
T-4 T-1-36633
6352
CUST.#332804-49

Figure 3-5

Reference beam Filter Holder

Figure 3-6 Slit-limited Resolution

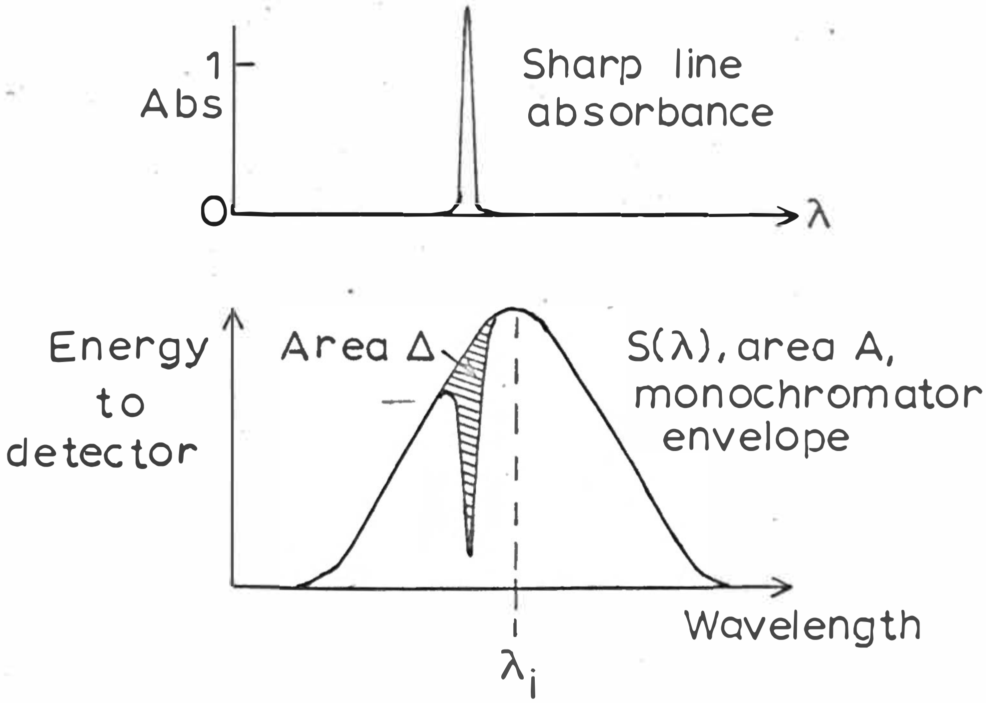


Figure 3-7 Quantitative Effect

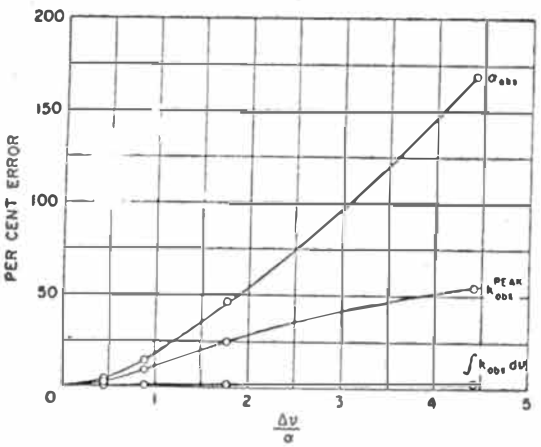


FIG. 1. Error made in direct measurement of line width, peak absorption coefficient, and line intensity as function of ratio of spectral slit width to line half-width for a single Lorentz line with 30% peak absorption and a Gauss slit function.

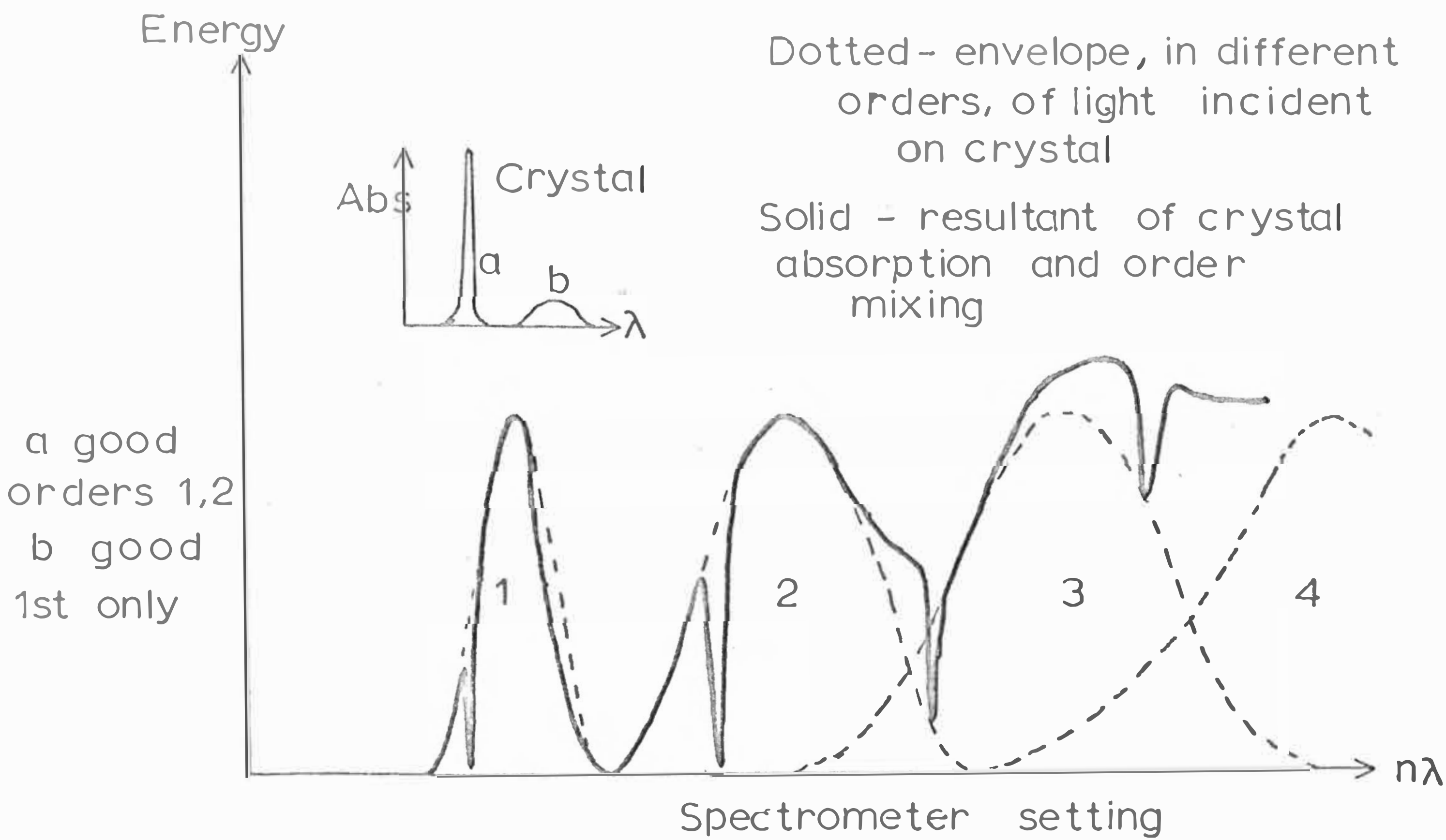
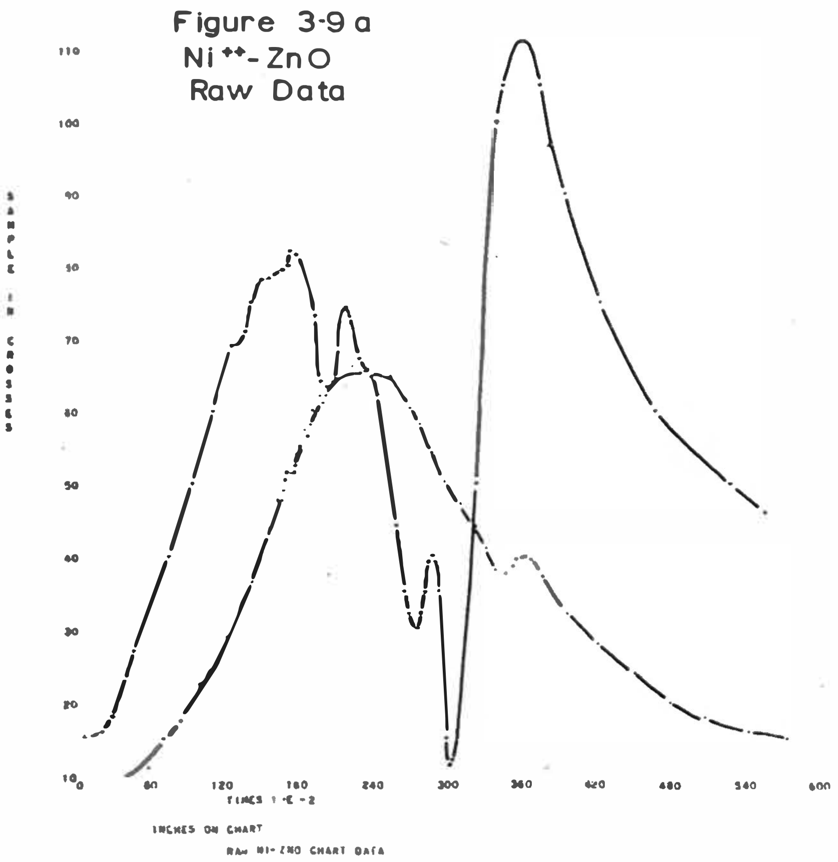
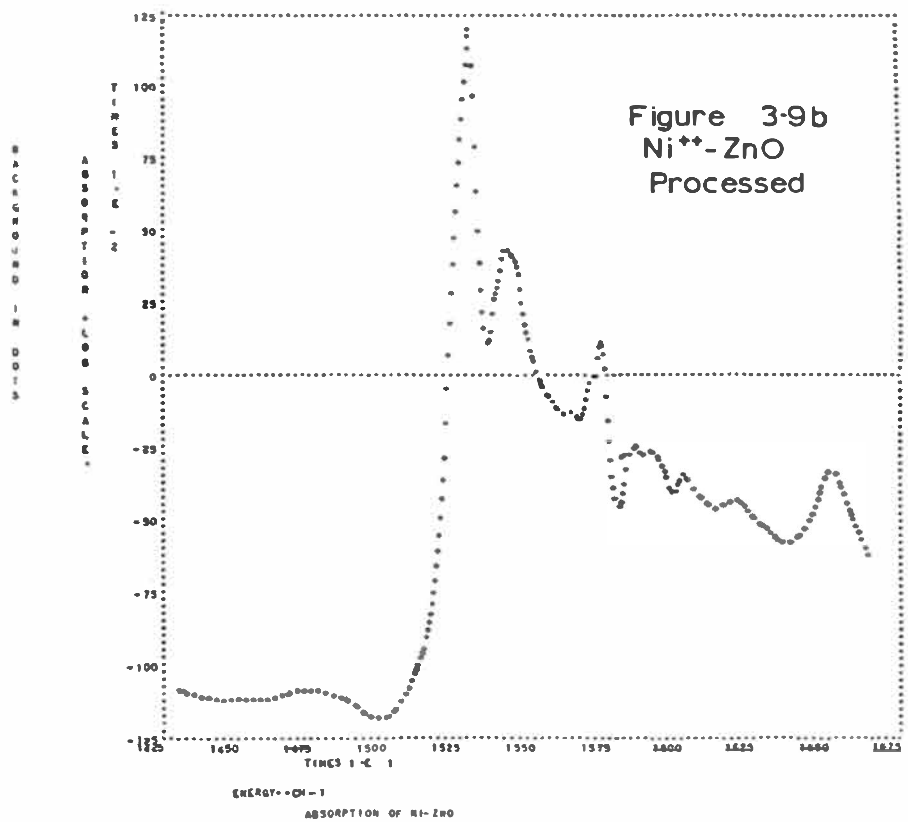


Figure 3-8 Overlapping Orders in Absorption

Figure 3-9 Ni - ZnO on Jarrell-Ash





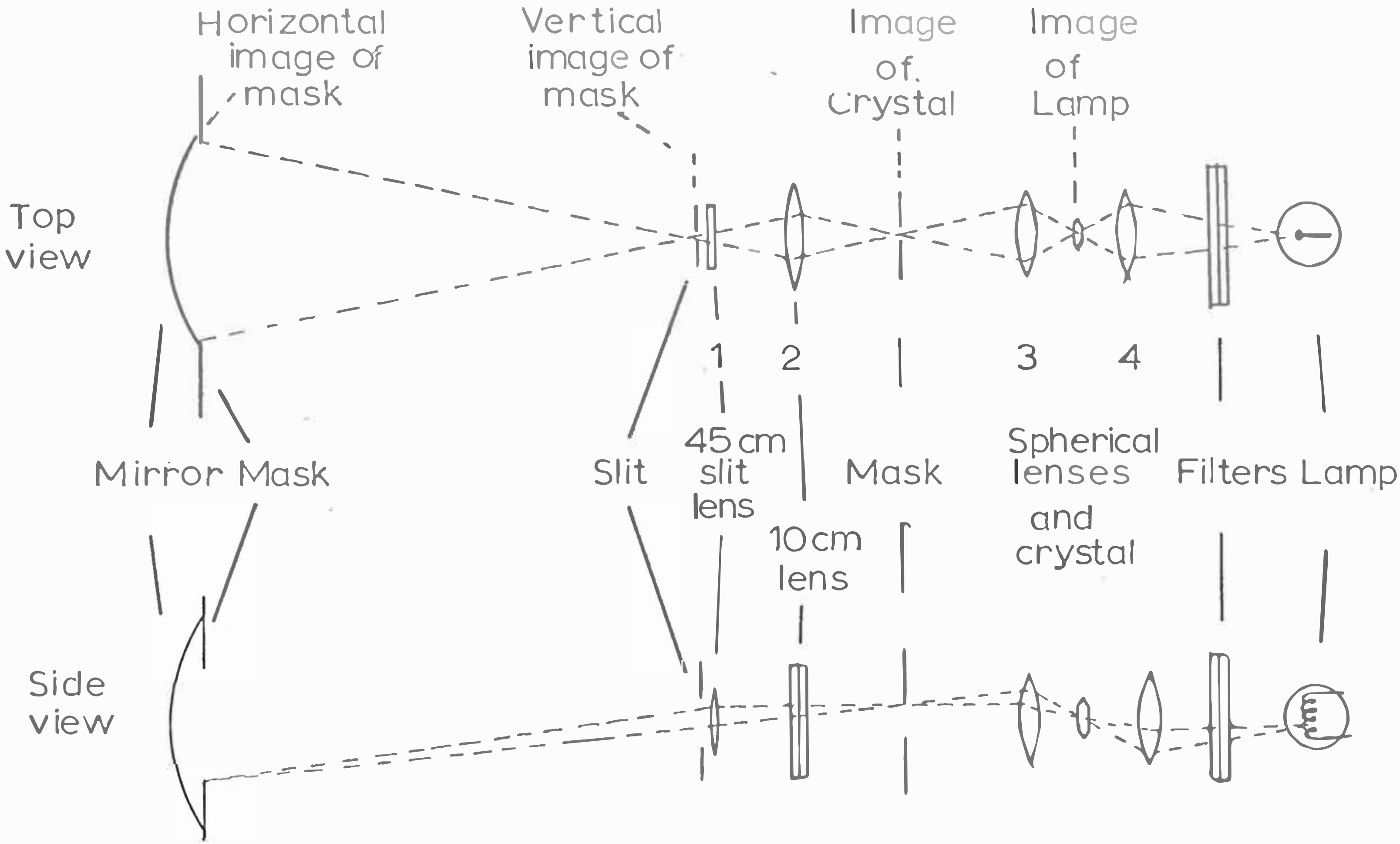


Figure 3-10 The Jarrell-Ash Condenser System

Figure 3-11 A Schematic Jarrell-Ash Chart

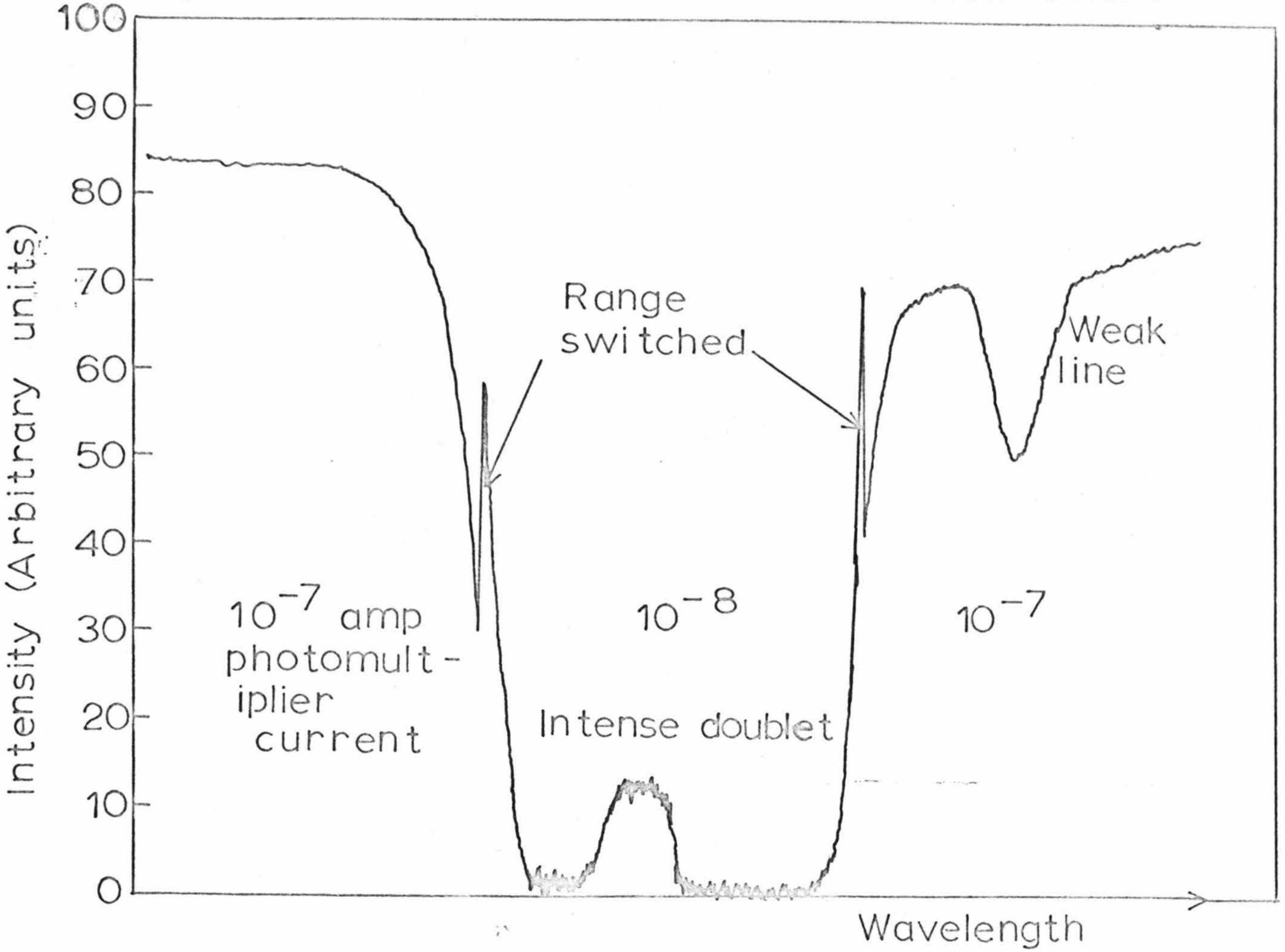
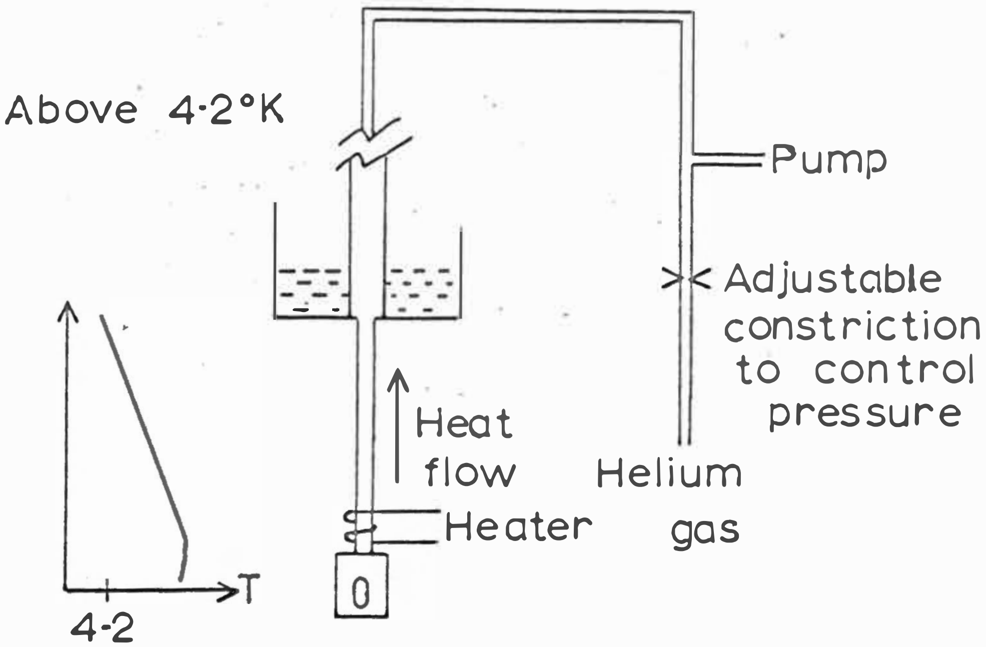
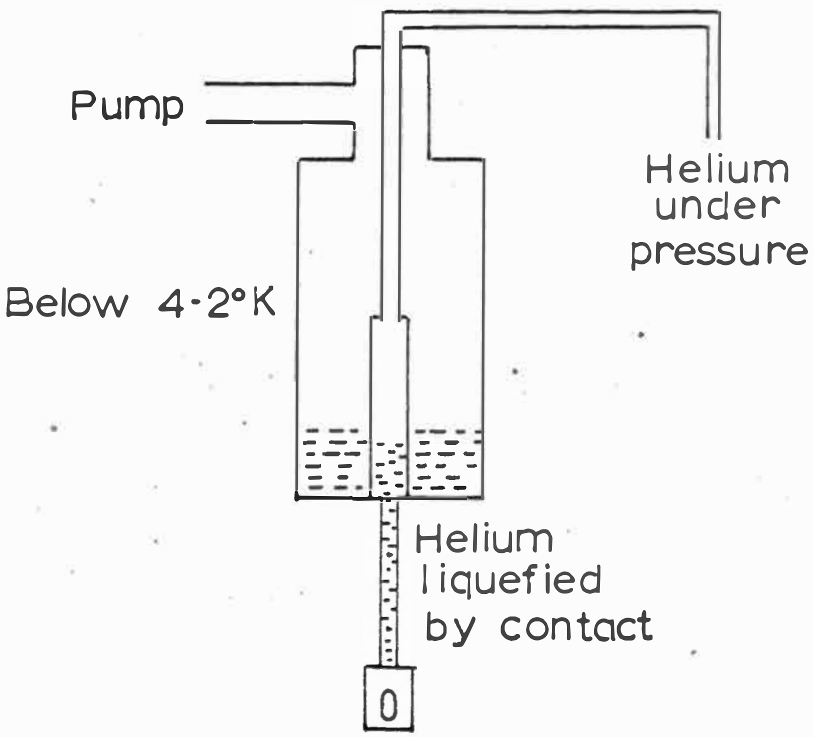


Figure 4-1 Andonian Dewar Operation





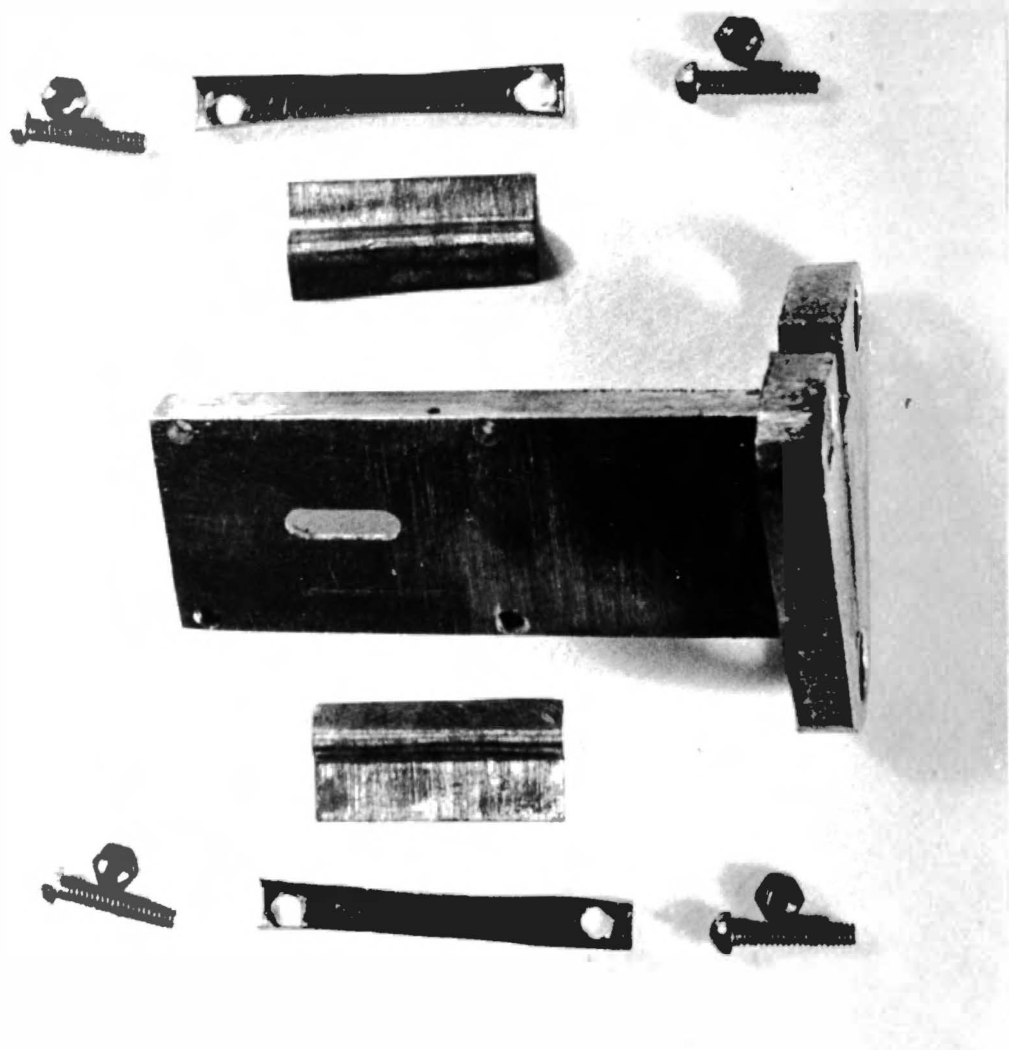


Figure 4·2

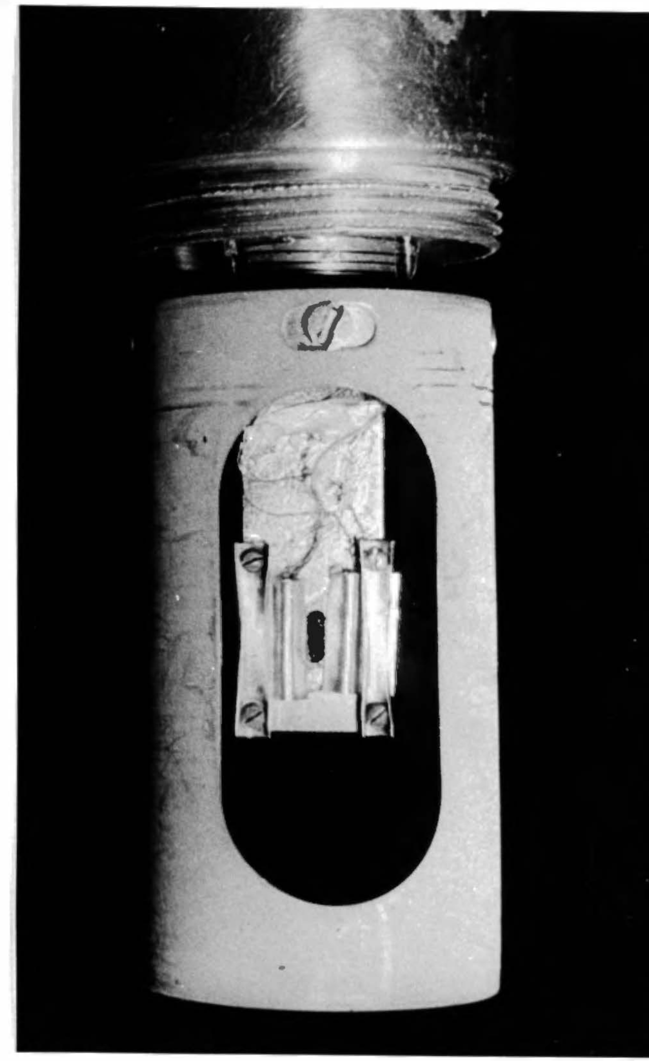


Figure 4·3

Sample holder disassembled and in position

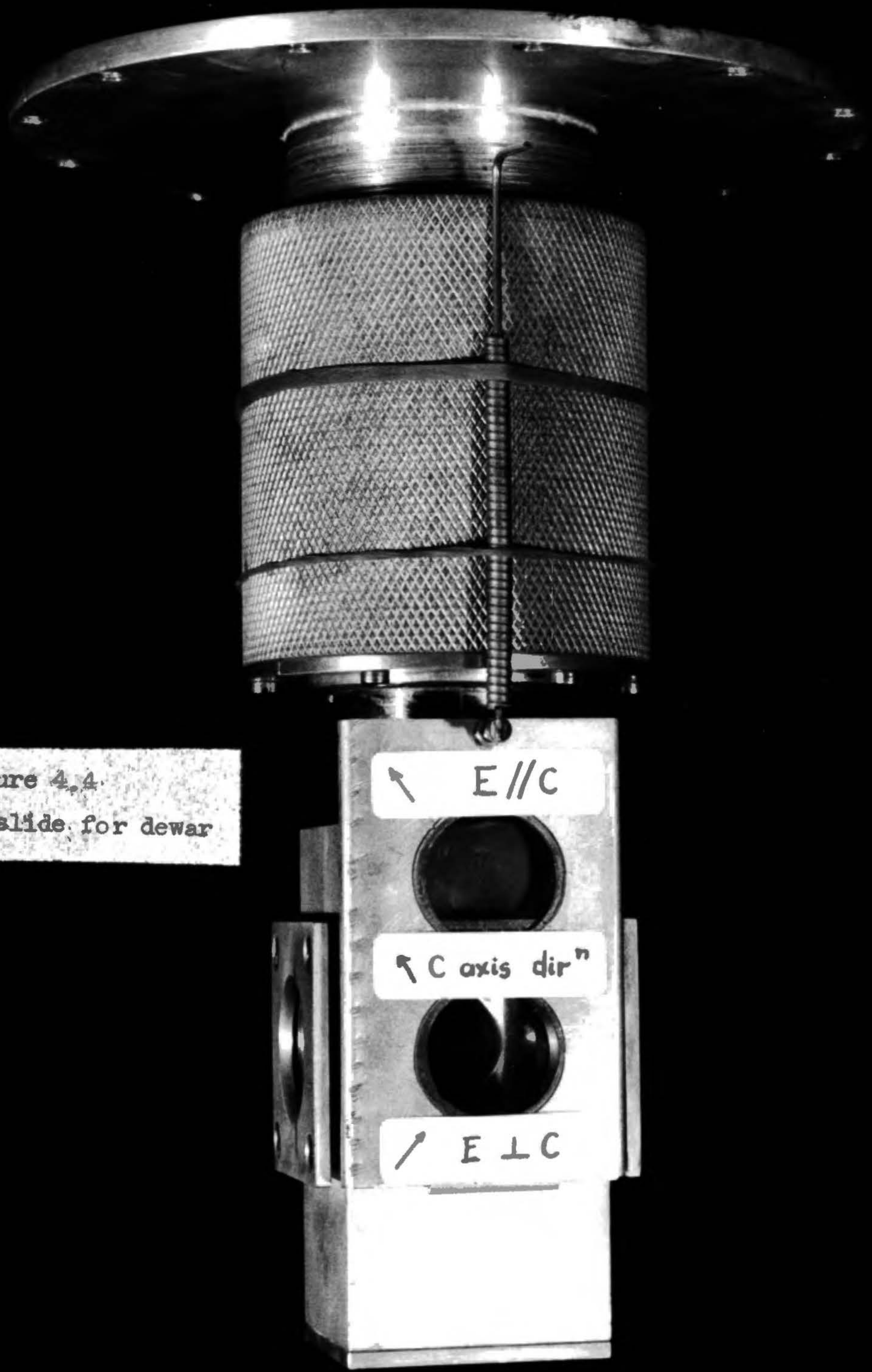


Figure 4.4
Polaroid slide for dewar

Figure 4·5 Polaroid Spectrum

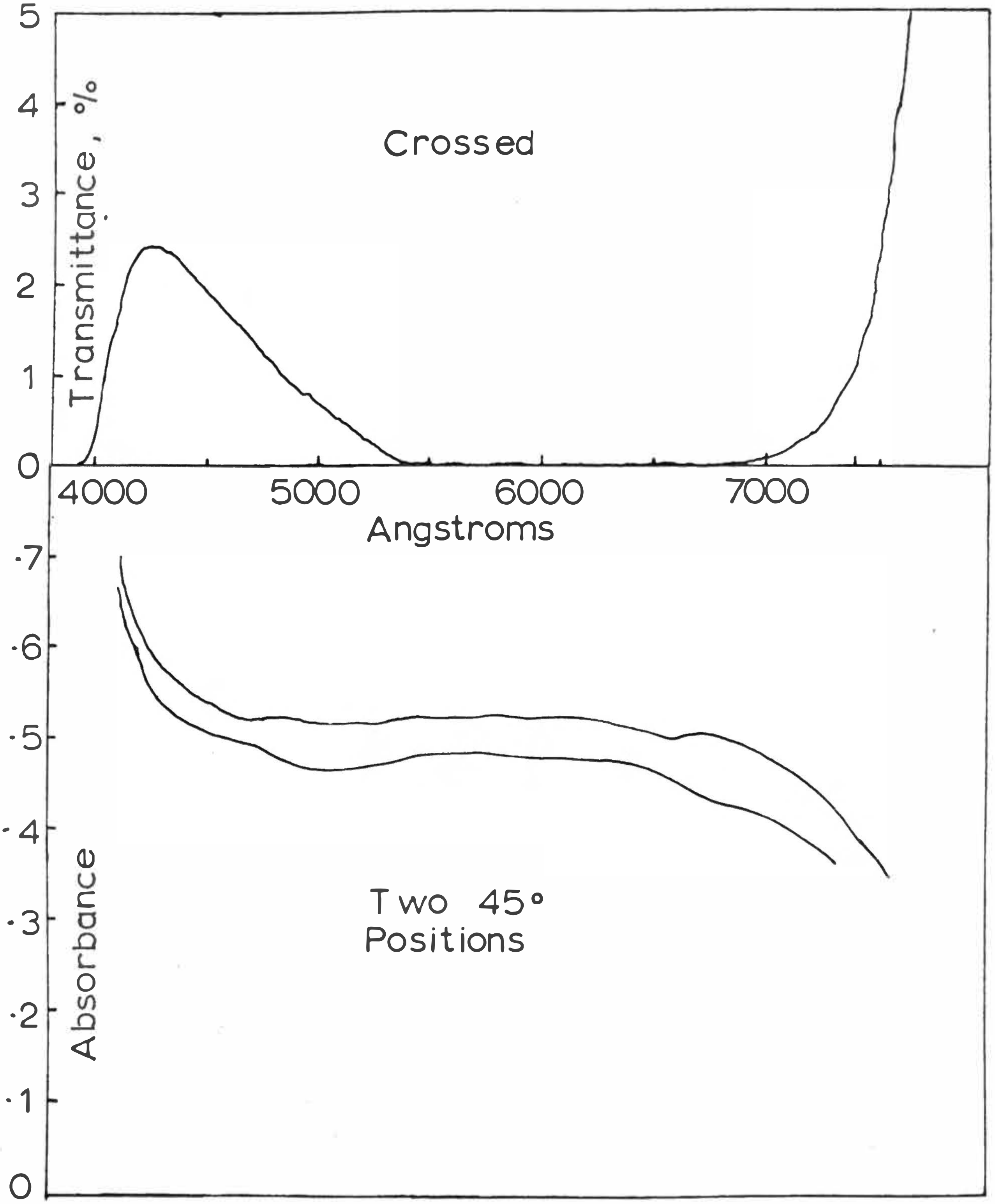
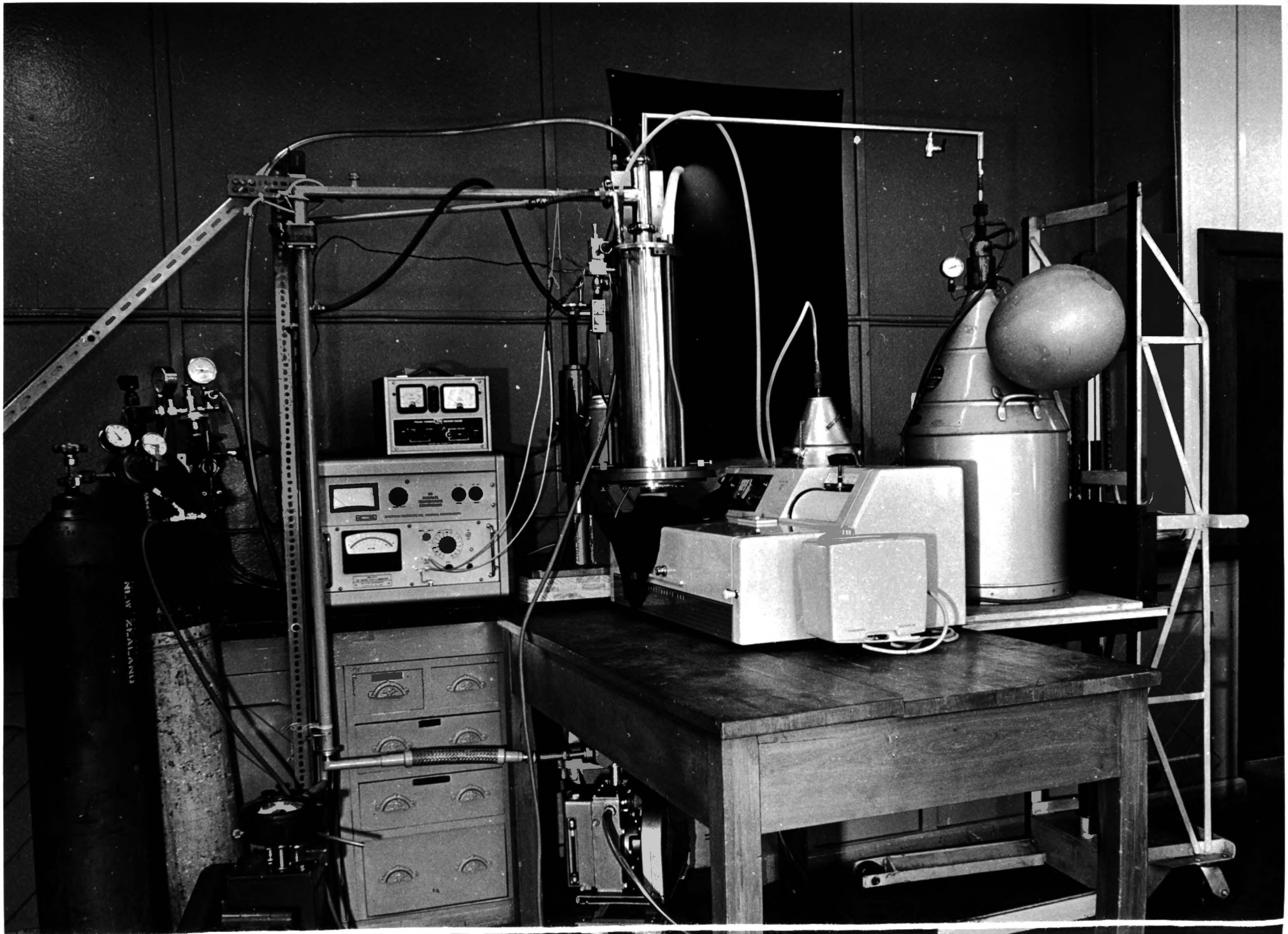


Figure 4.6

Bausch and Lomb Dewar Assembly


NEW ZEALAND

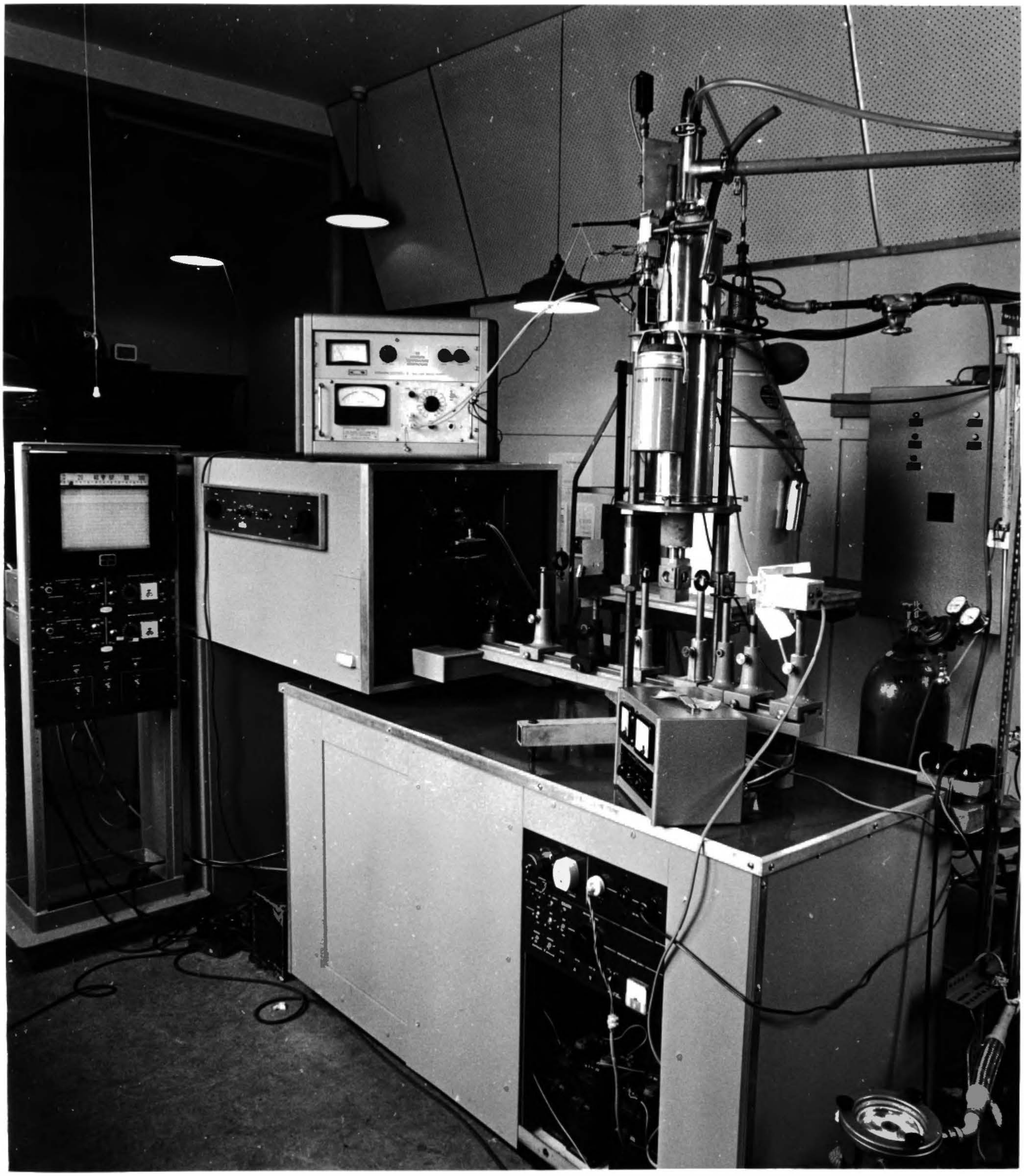


Figure 4-7 Jarrell-Ash Assembly

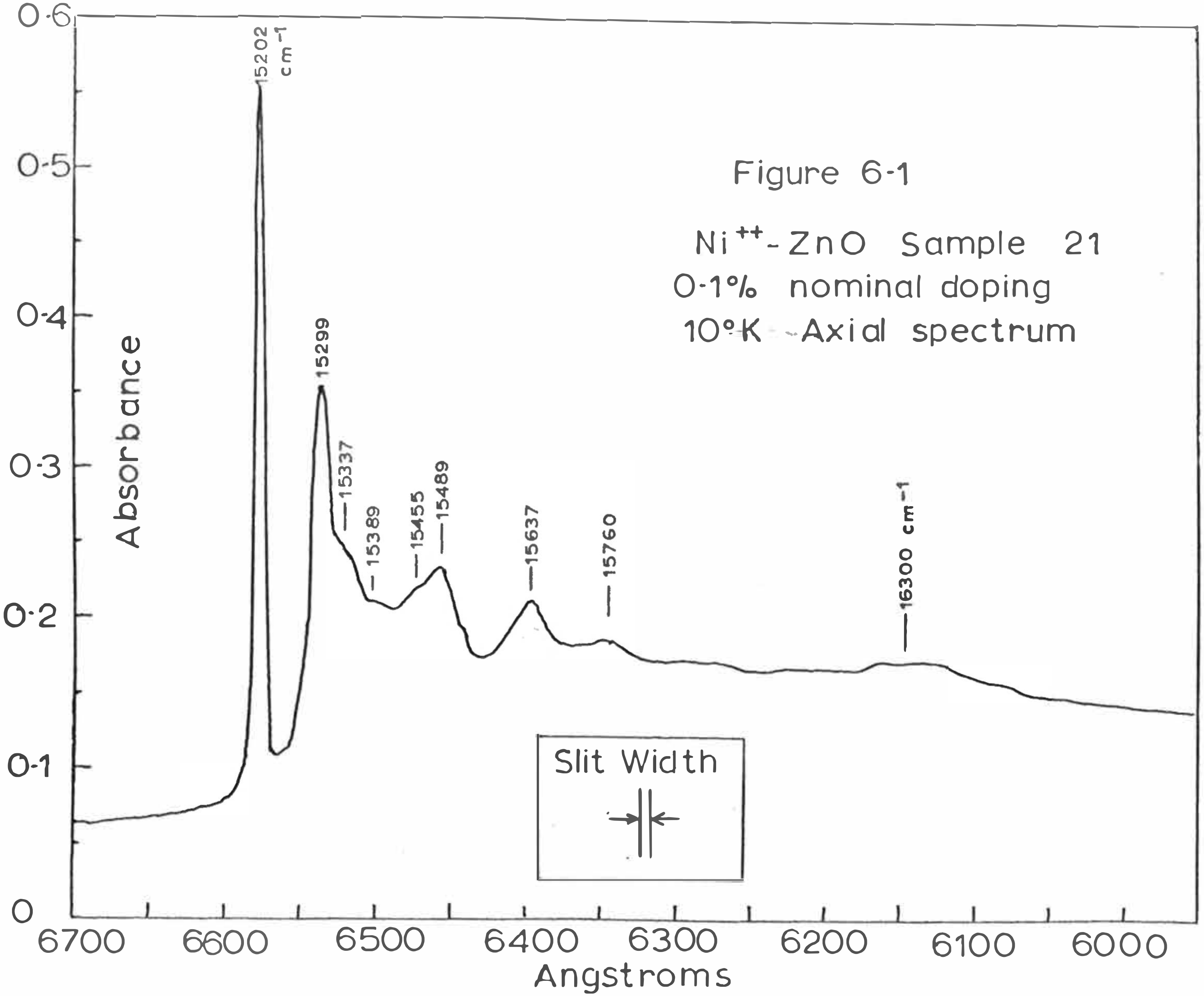
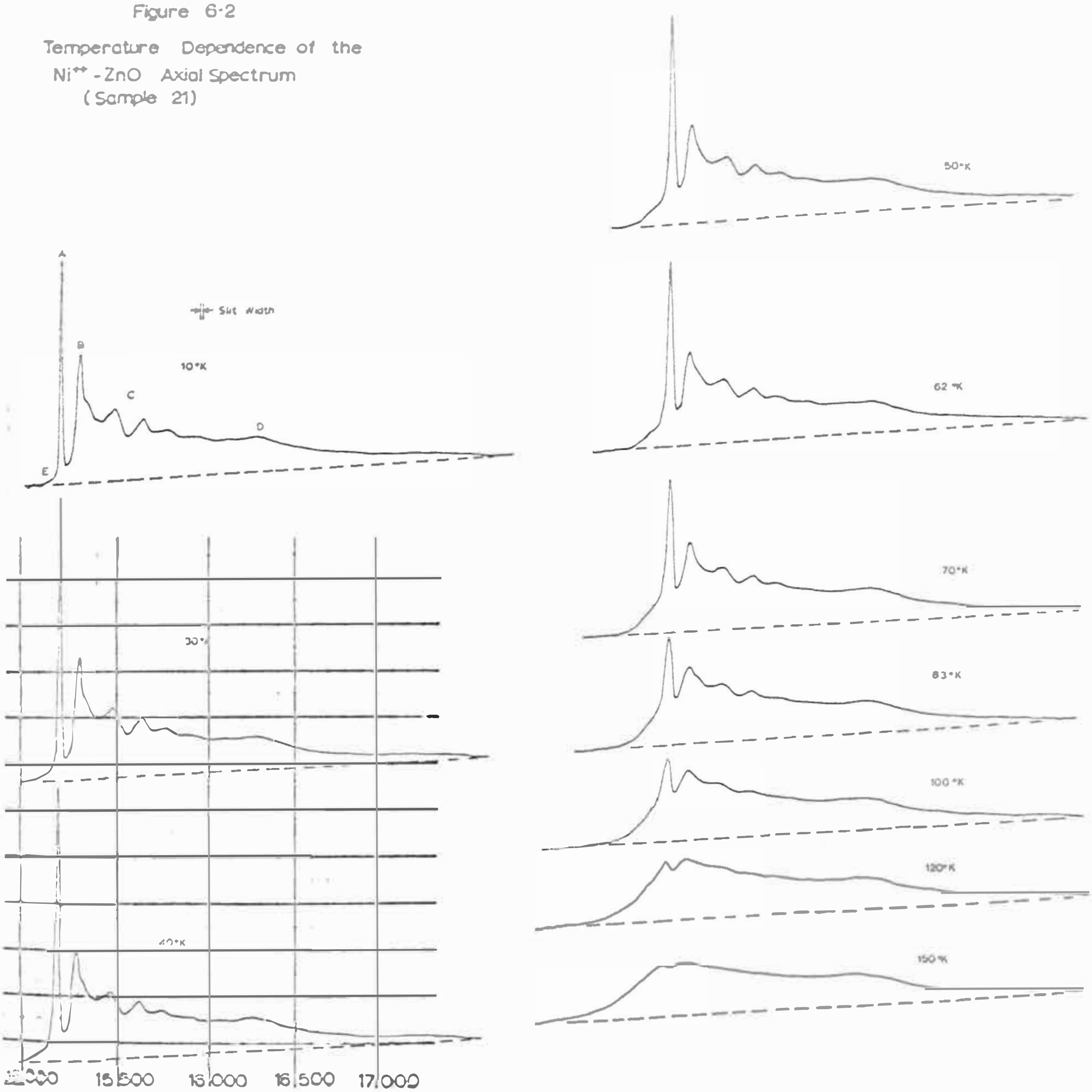
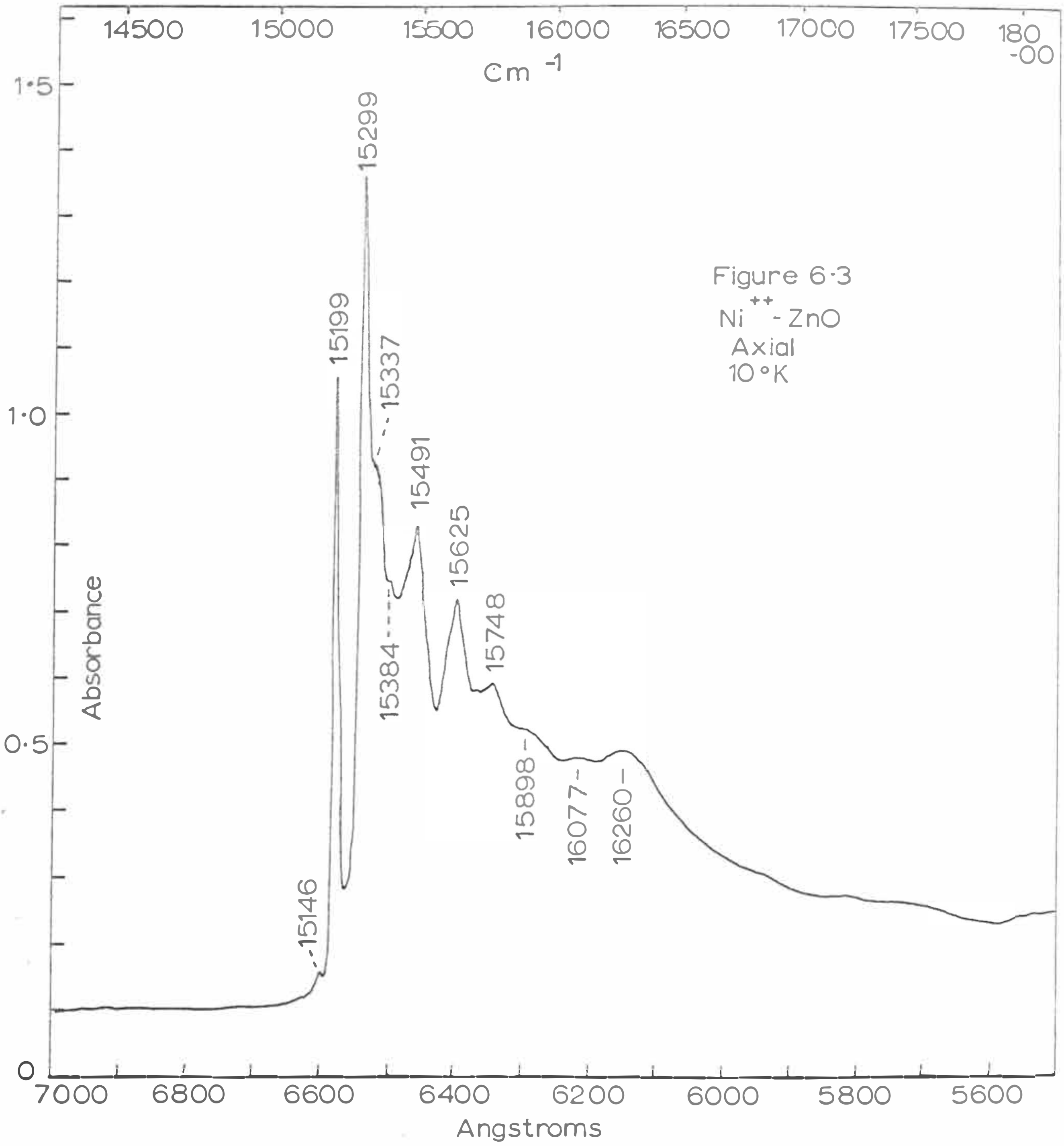


Figure 6-1
Ni^{++}-ZnO Sample 21
0·1% nominal doping
10°K Axial spectrum
Absorbance
Angstroms
15202 cm^{-1}
15299
15337
15389
15455
15489
15637
15760
16300 cm^{-1}
Slit Width
0·6
0·5
0·4
0·3
0·2
0·1
0
6700
6600
6500
6400
6300
6200
6100
6000

Figure 6·2

Temperature Dependence of the Ni^{++} - ZnO Axial Spectrum (Sample 21)




14500
15000
15500
16000
16500
17000
17500
180
-00
Cm -1
1·5
1·0
0·5
0
Absorbance
15299
15199
15337
15491
15625
15384
15748
15898
16077
16260
15146
Figure 6-3
Ni ++ - ZnO
Axial
10 °K
7000
6800
6600
6400
6200
6000
5800
5600
Angstroms

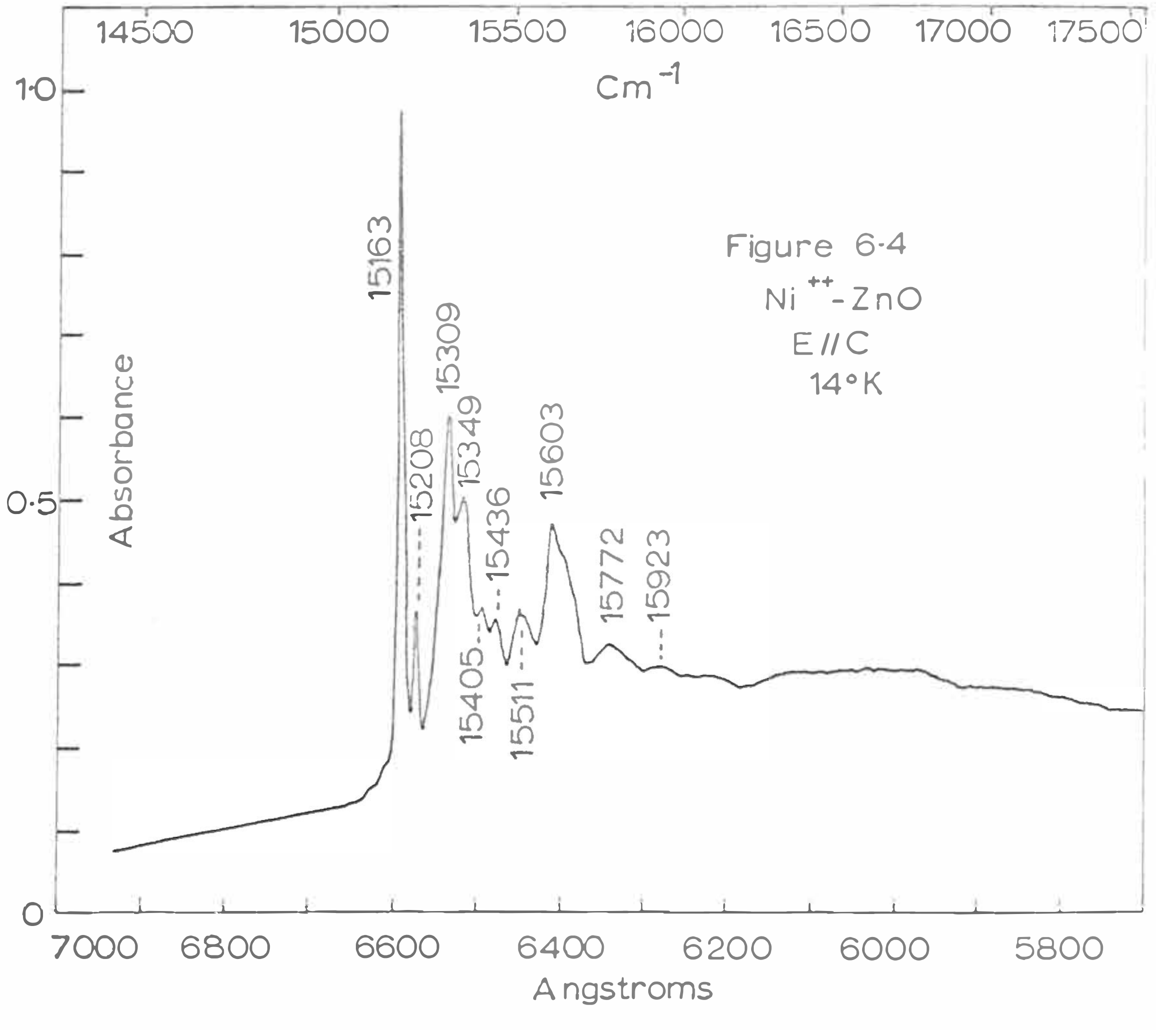
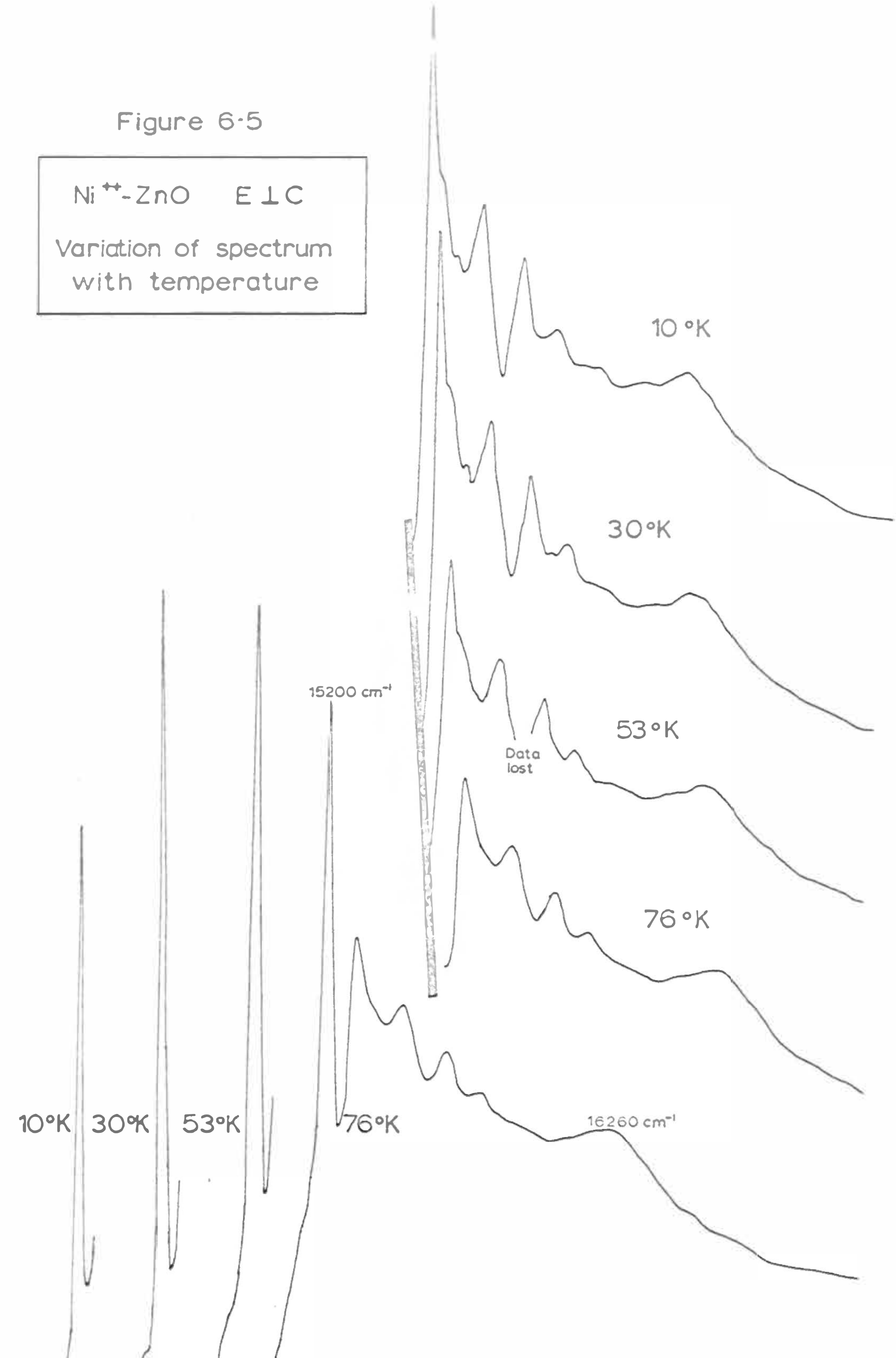
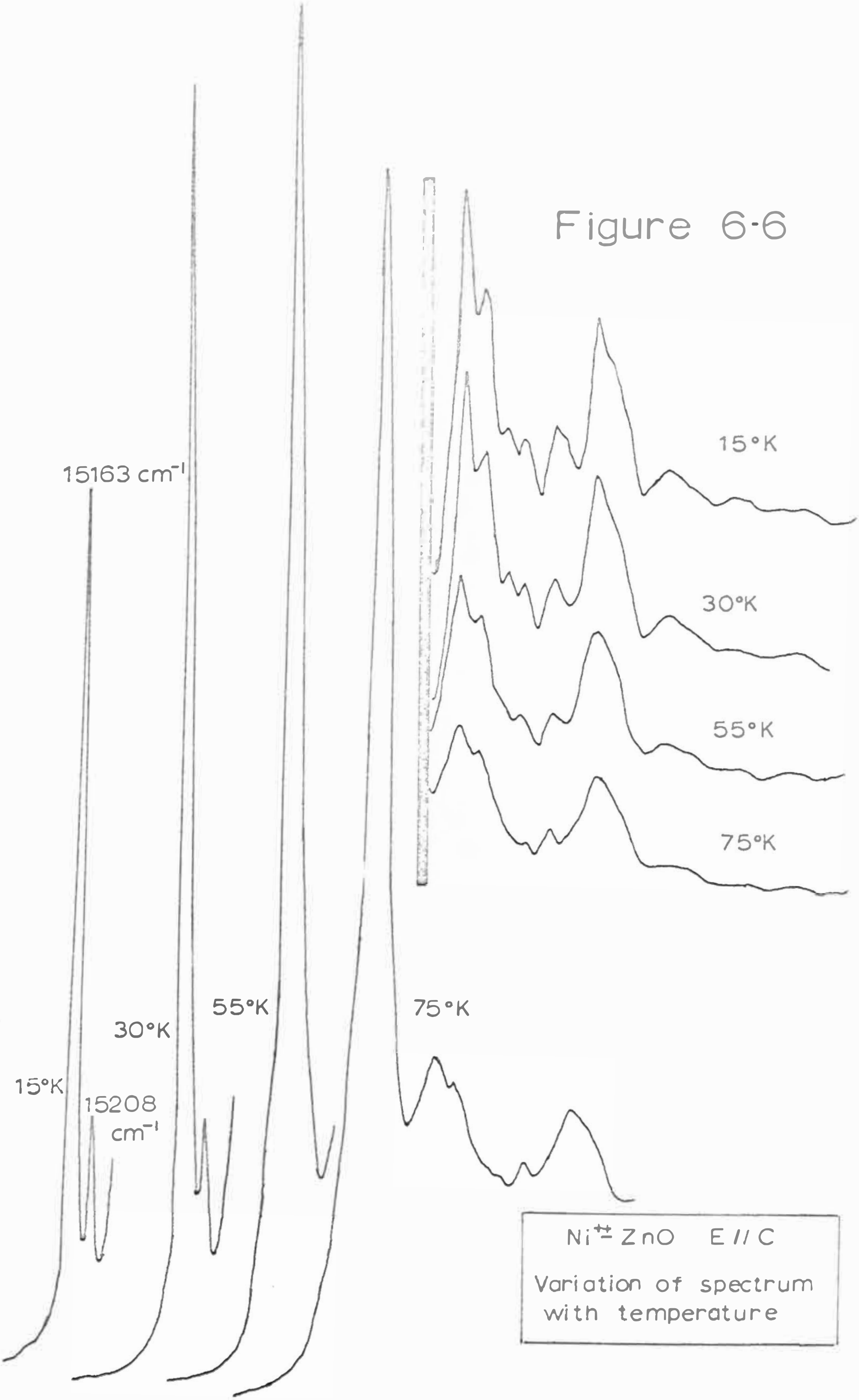

14500
15000
15500
16000
16500
17000
17500
Cm^{-1}
1·0
0·5
0
Absorbance
15163
15208
15309
15349
15405
15436
15511
15603
15772
15923
Figure 6·4
Ni^{++}-ZnO
E//C
14°K
7000
6800
6600
6400
6200
6000
5800
Angstroms

Figure 6-5

Ni^{++}-ZnO E⊥C

Variation of spectrum with temperature





15163 cm⁻¹
15°K
15208 cm⁻¹
30°K
55°K
75°K
15°K
30°K
55°K
75°K
Ni++ ZnO E // C
Variation of spectrum with temperature

Figure 6-6

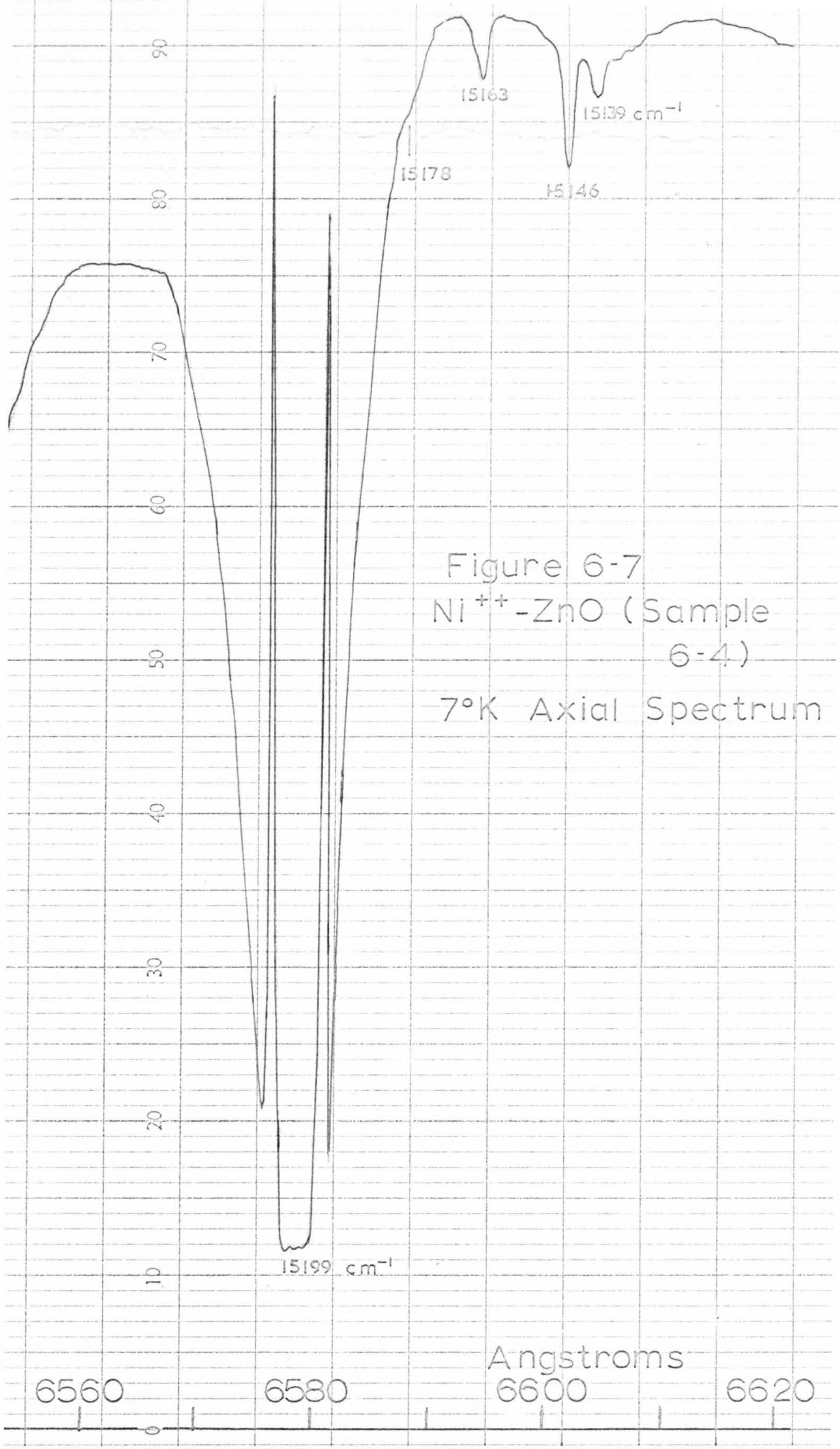


Figure 6-7
Ni^{++}-ZnO (Sample 6-4)
7°K Axial Spectrum

Figure 6-8 Ni^{++}-ZnO Axial Spectrum (Jarrell-Ash)

(Sample 6-1)

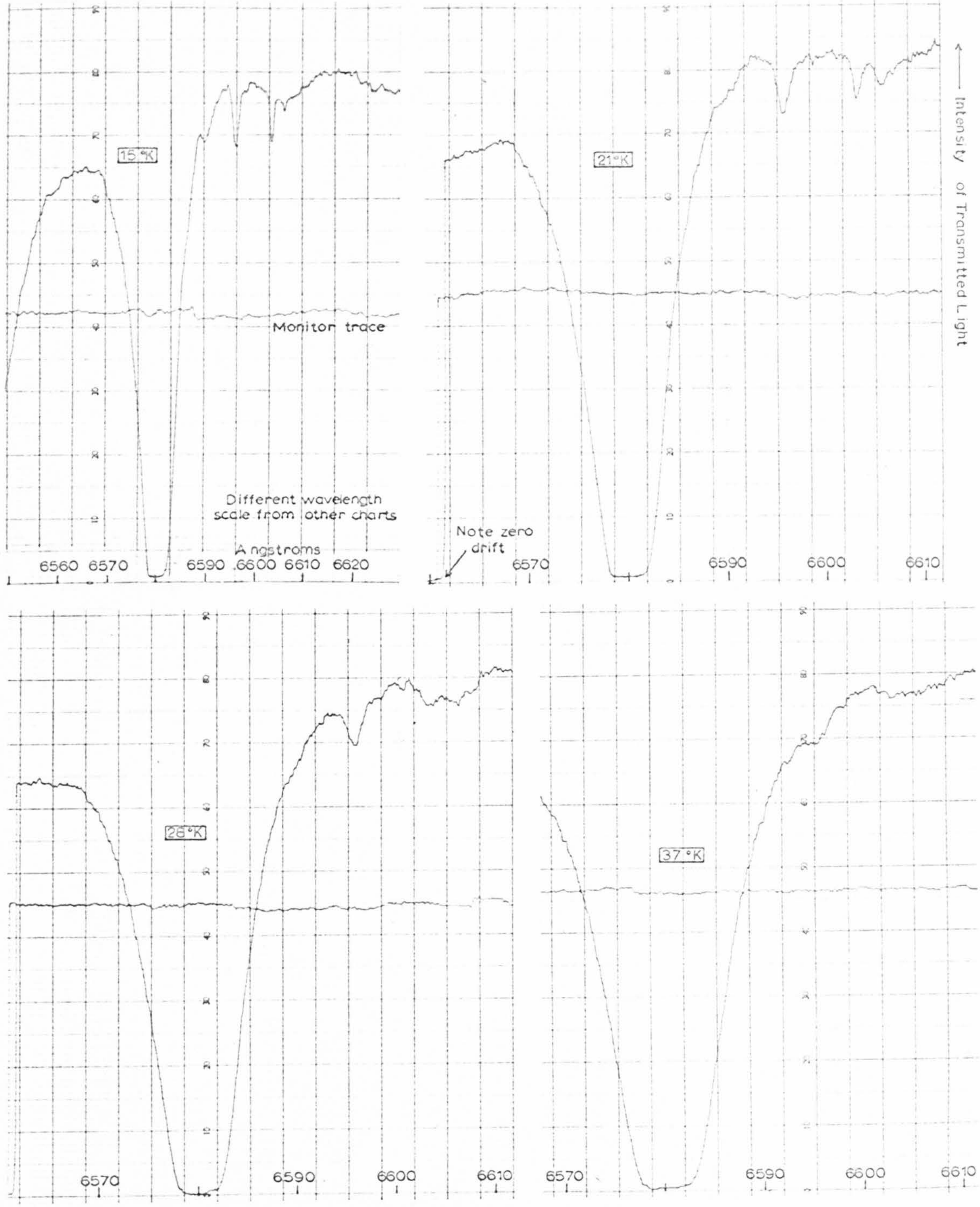
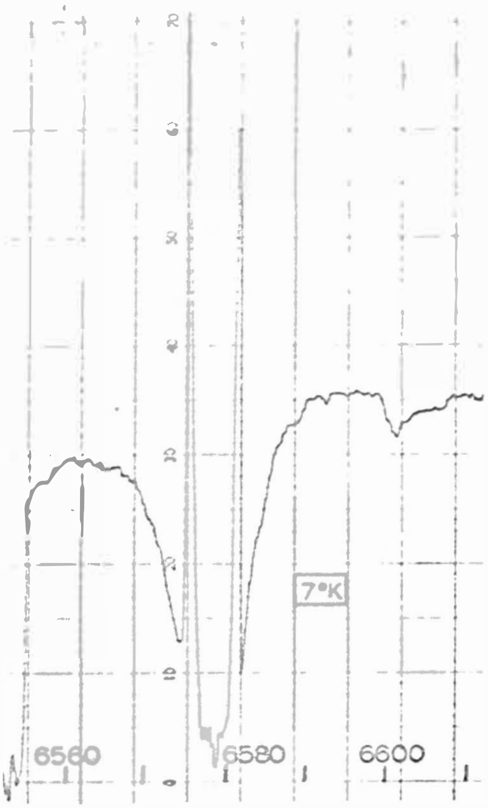
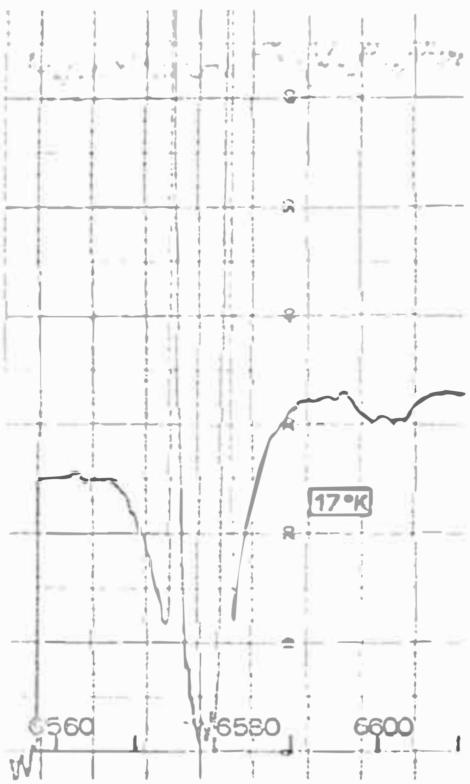


Figure 6-9 Ni^{++}-ZnO

J-A Sigma Spectrum

30°K trace on higher sensitivity





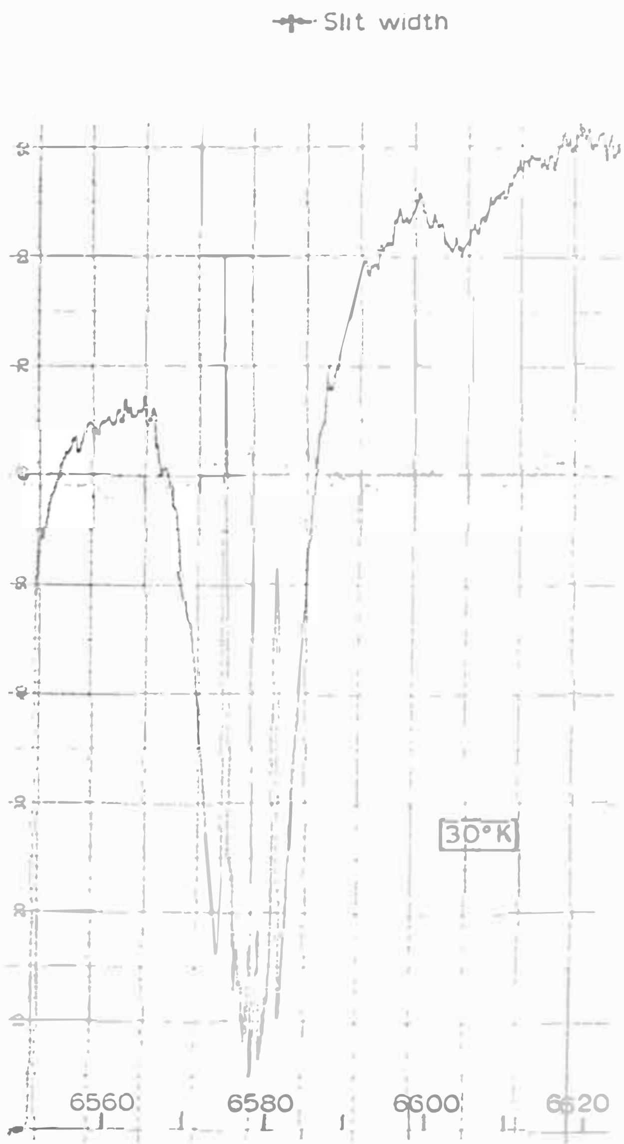
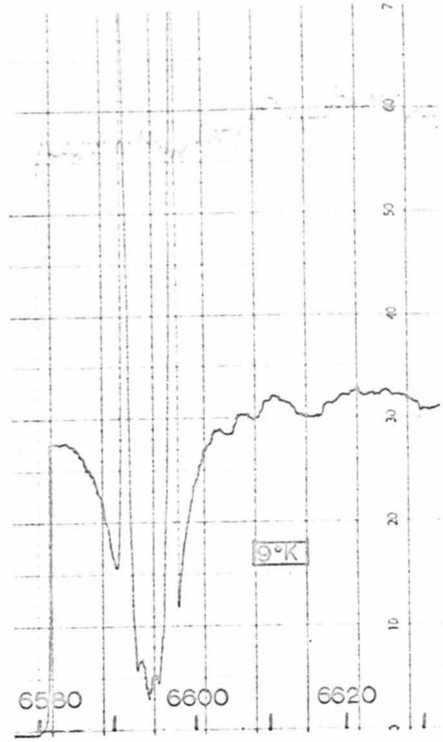


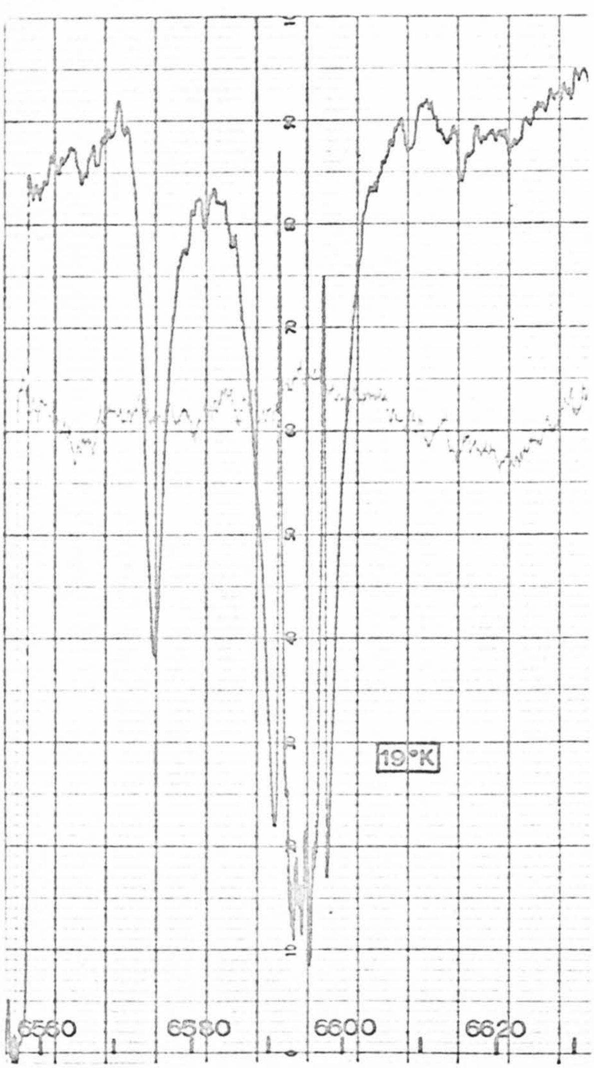
Figure 6-10 Ni^{++}-ZnO

J–A Pi Spectrum

9°K trace on lower sensitivity, 15207 cm^{-1} line not recorded

—|— Slit width





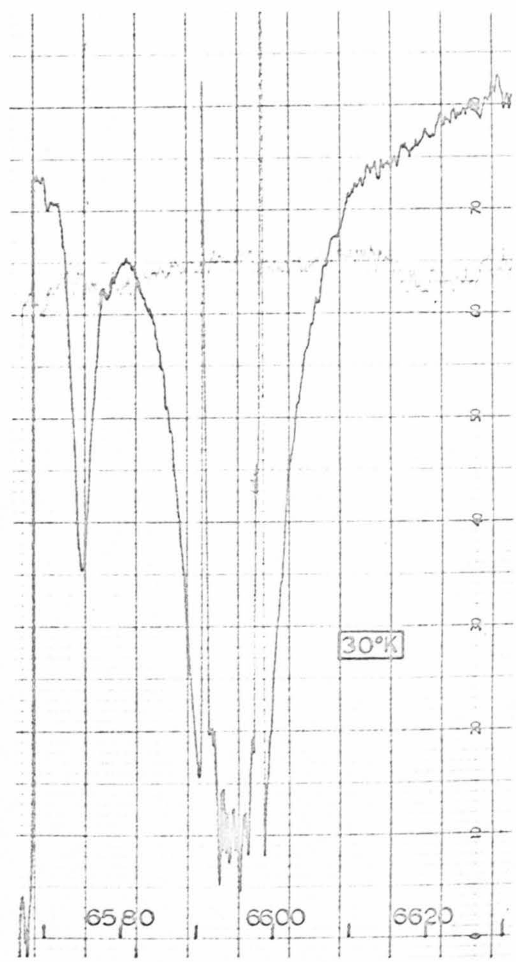


Figure 6-11 Histograms of Spectral Components for two different Ni^{++} Dopings

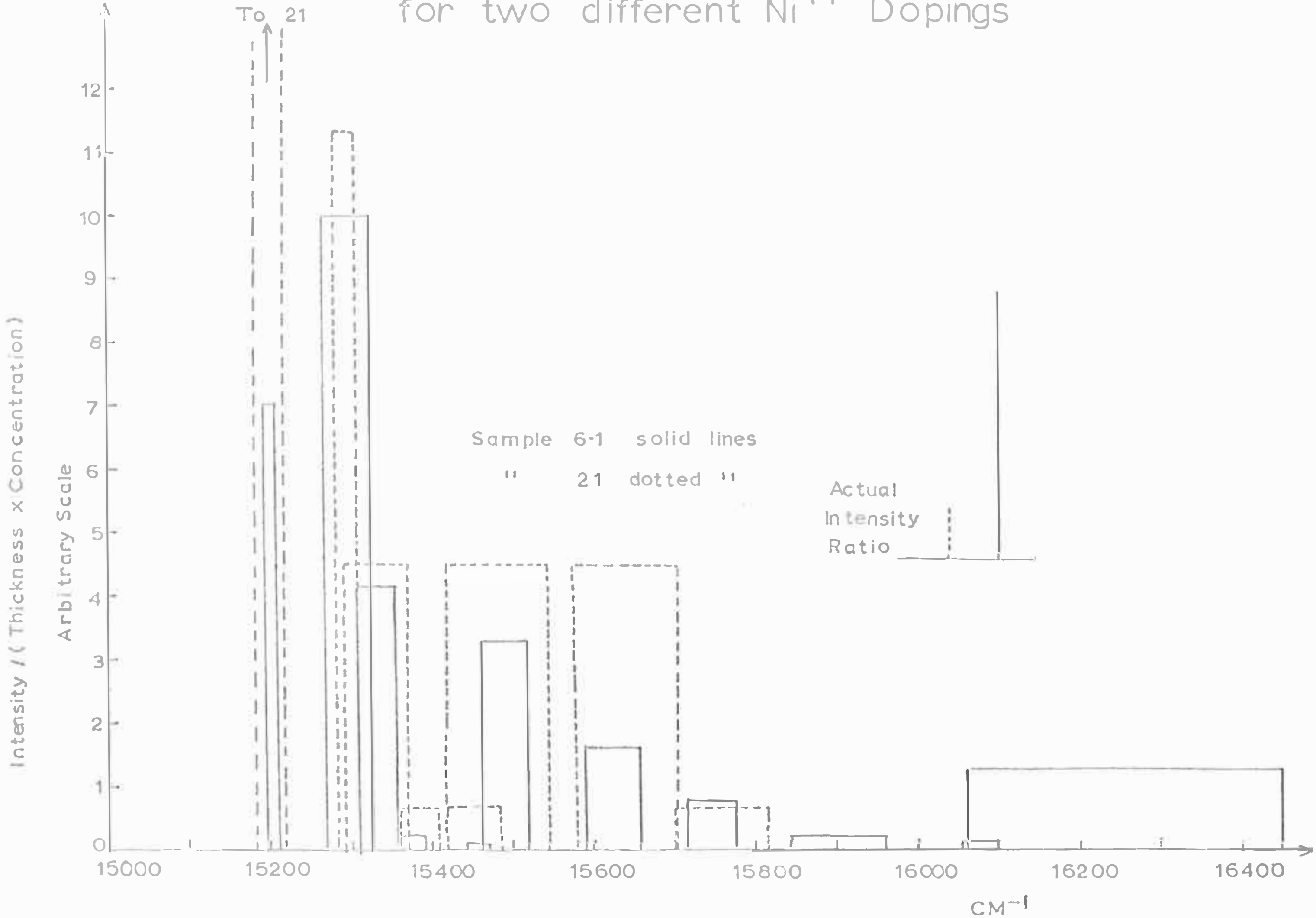


Figure 6-12 Concentration Dependence of Weak Lines (Jarrell-Ash)

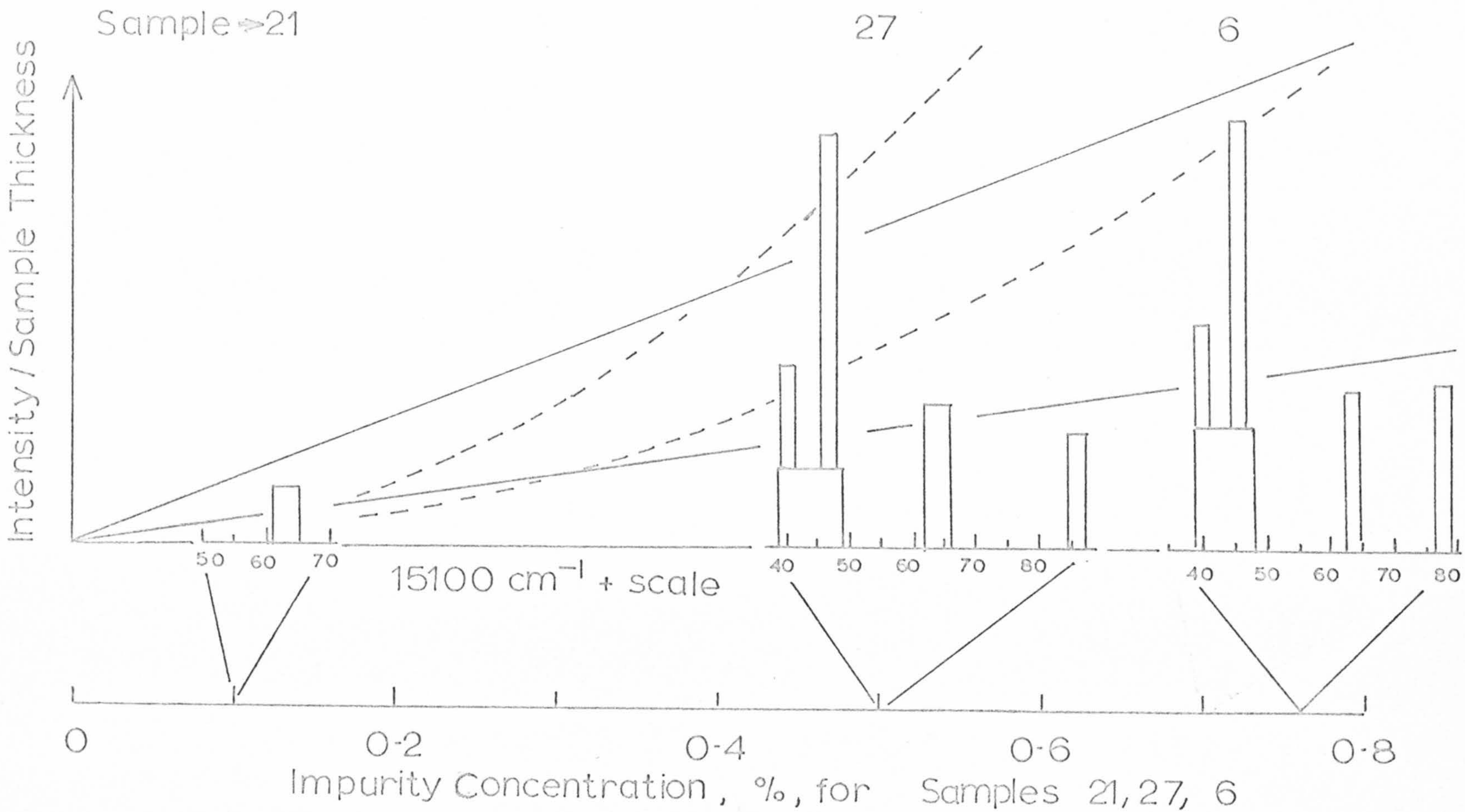


Figure 6-13 Sharp Line Temperature Dependence (J-A)

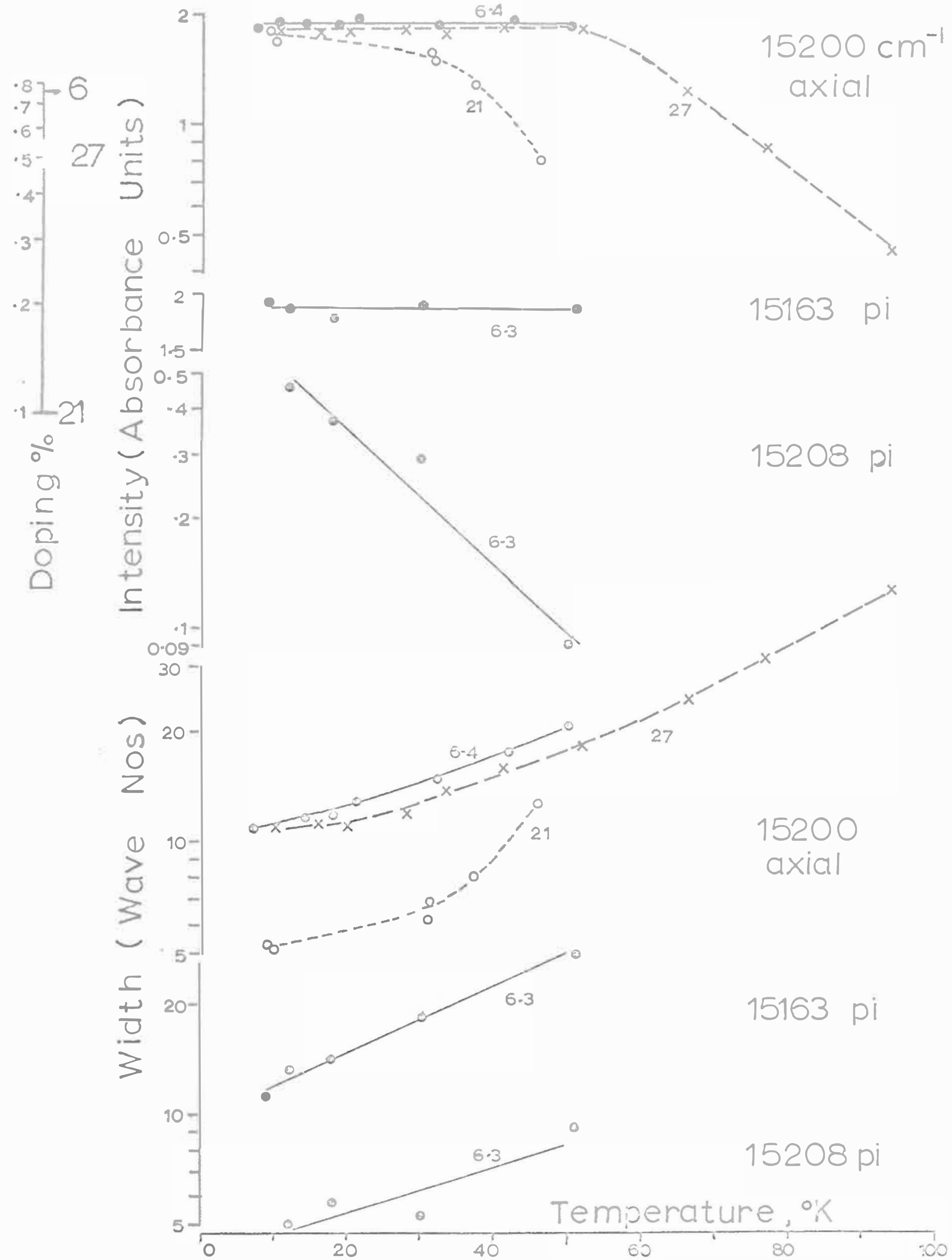


Figure 6-14 Temperature Dependence of Sharp Line Areas (J-A)

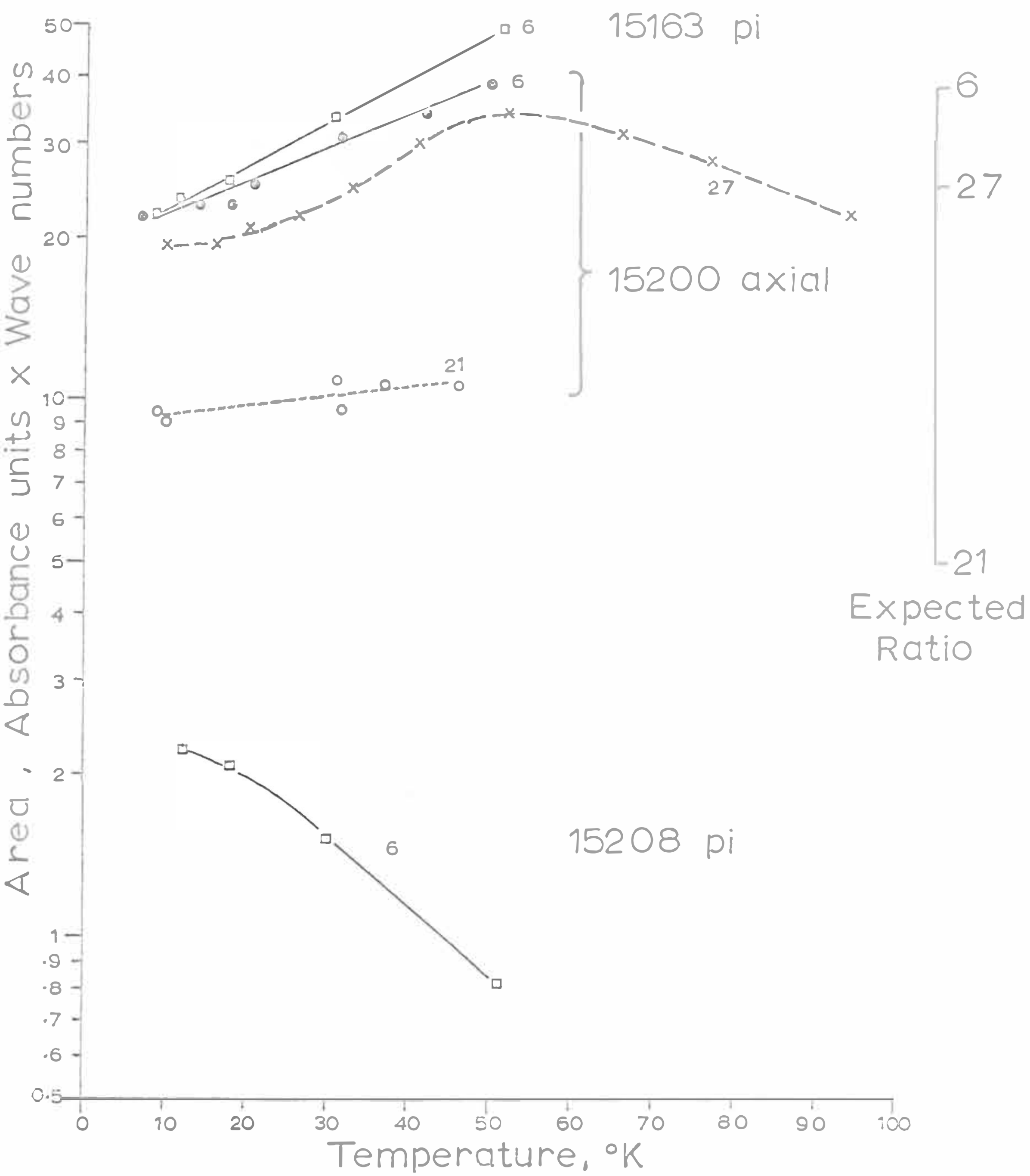
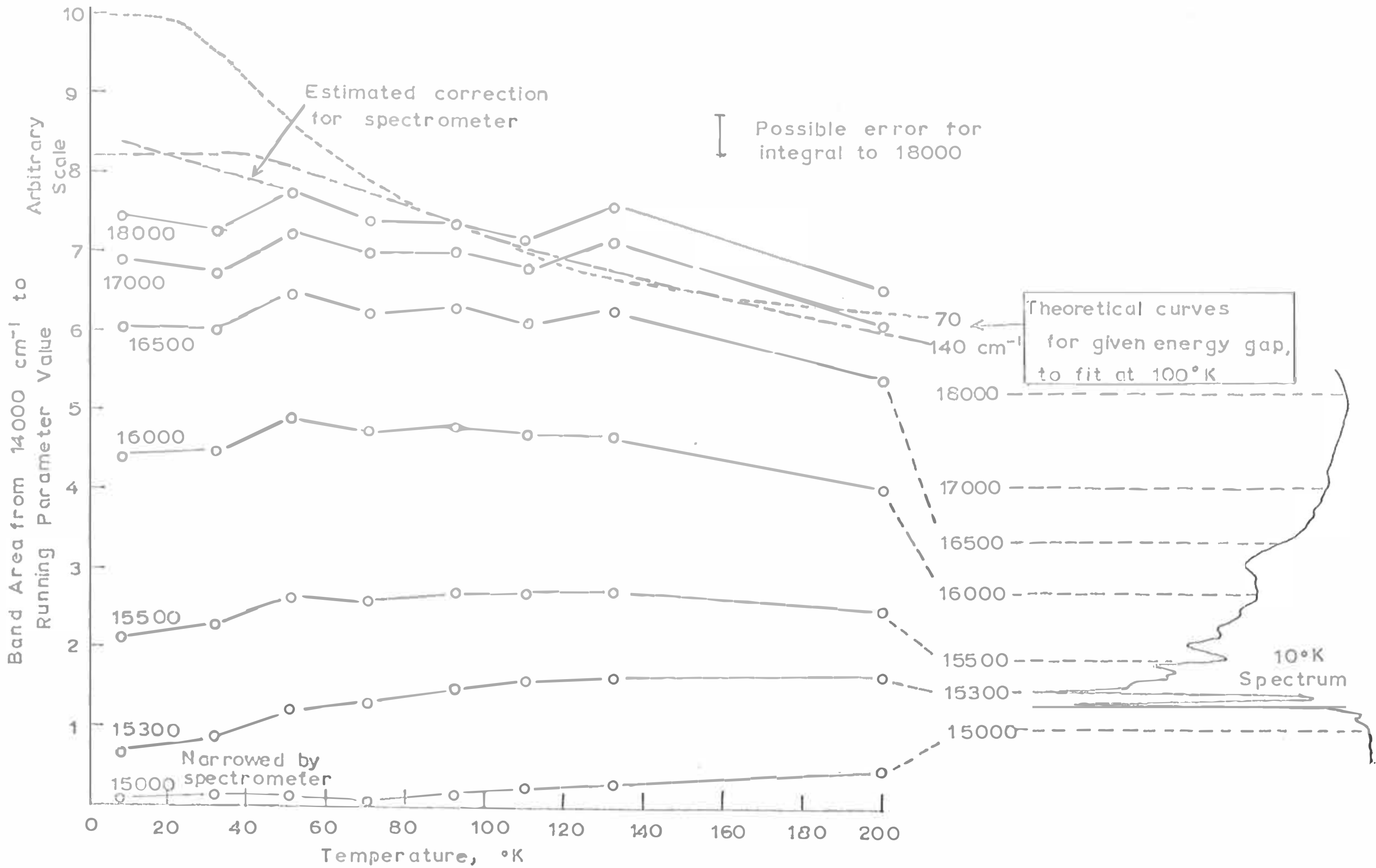


Figure 6.15 Total Integrated Absorption of Ni^{++}-ZnO Visible Band



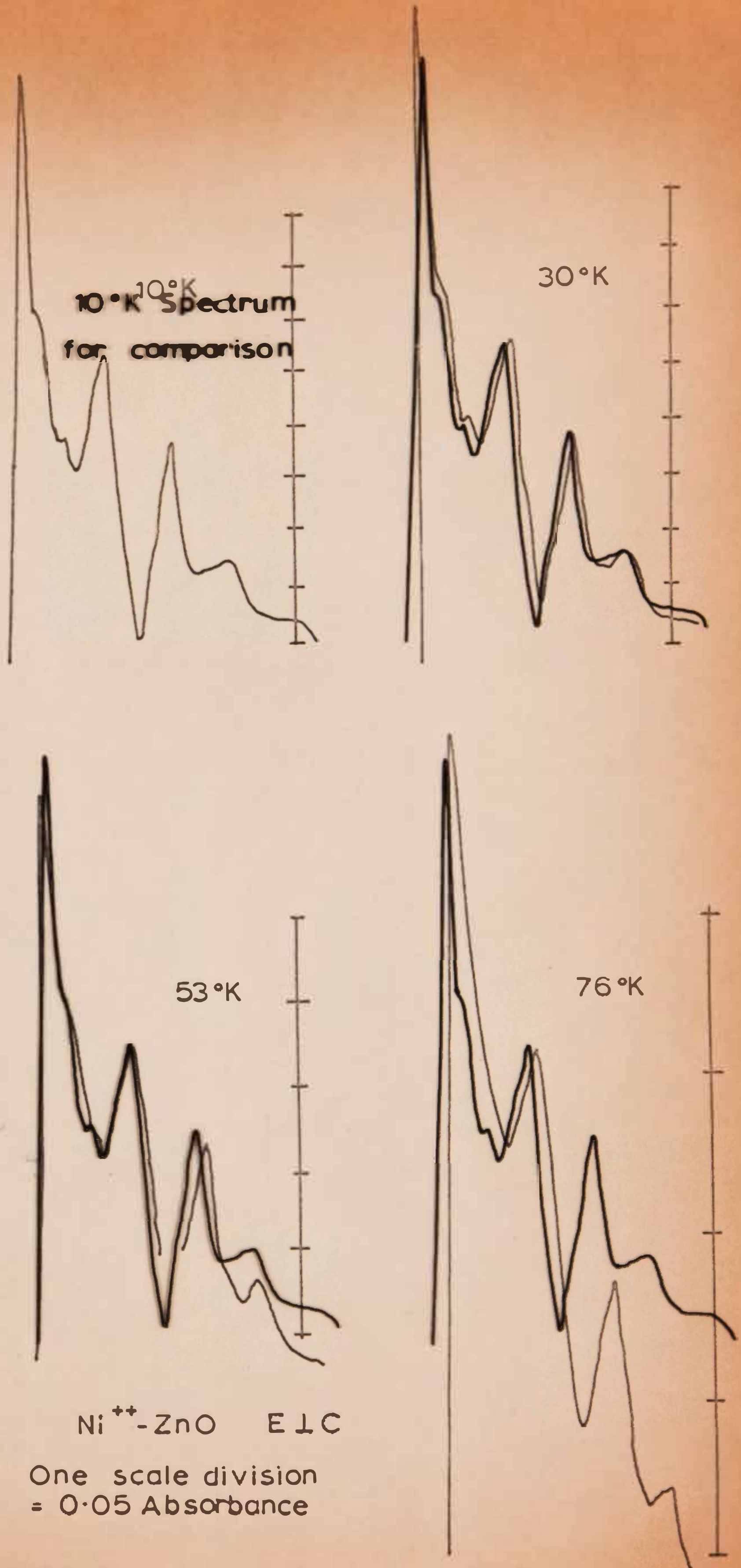
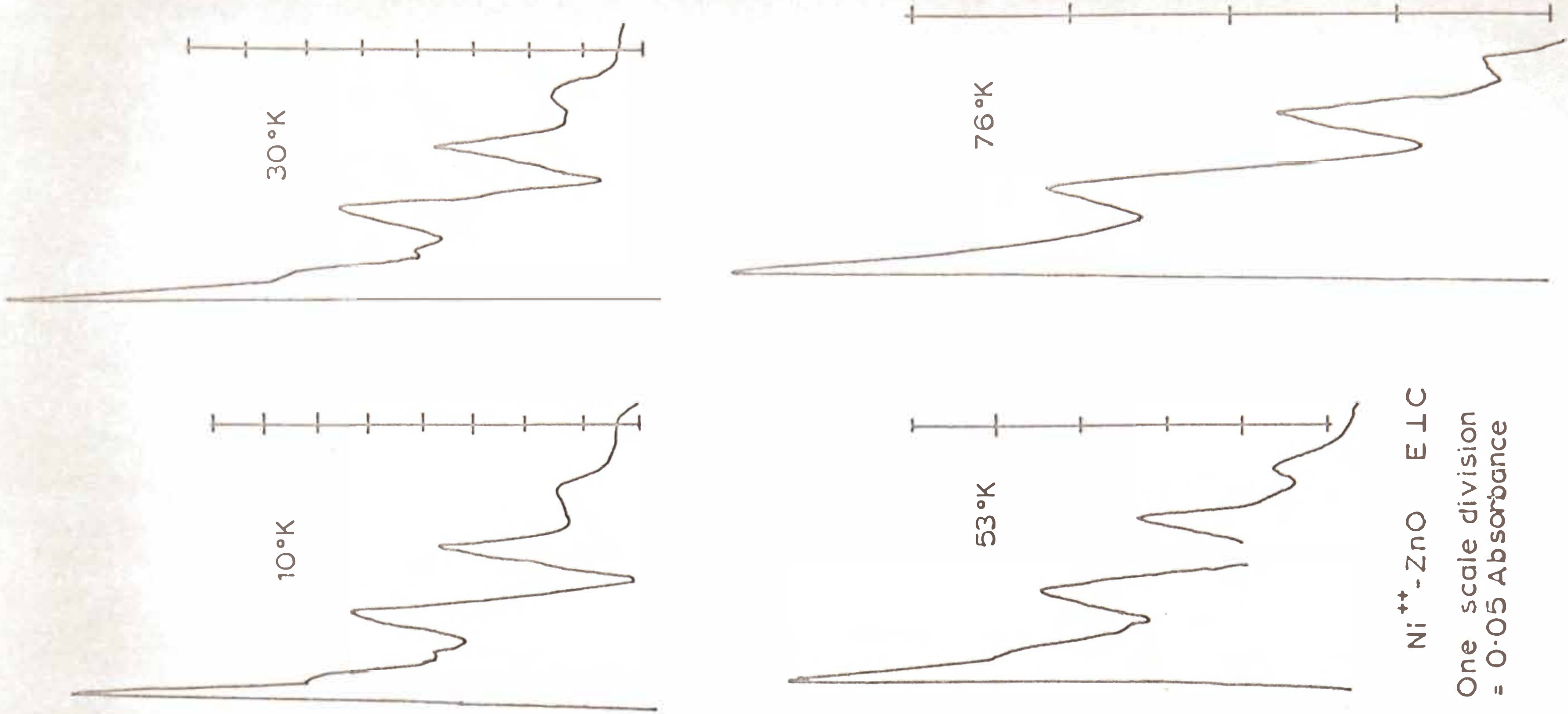


Figure 6·16 Band Shape Fitting Ni^{++}-ZnO Sigma

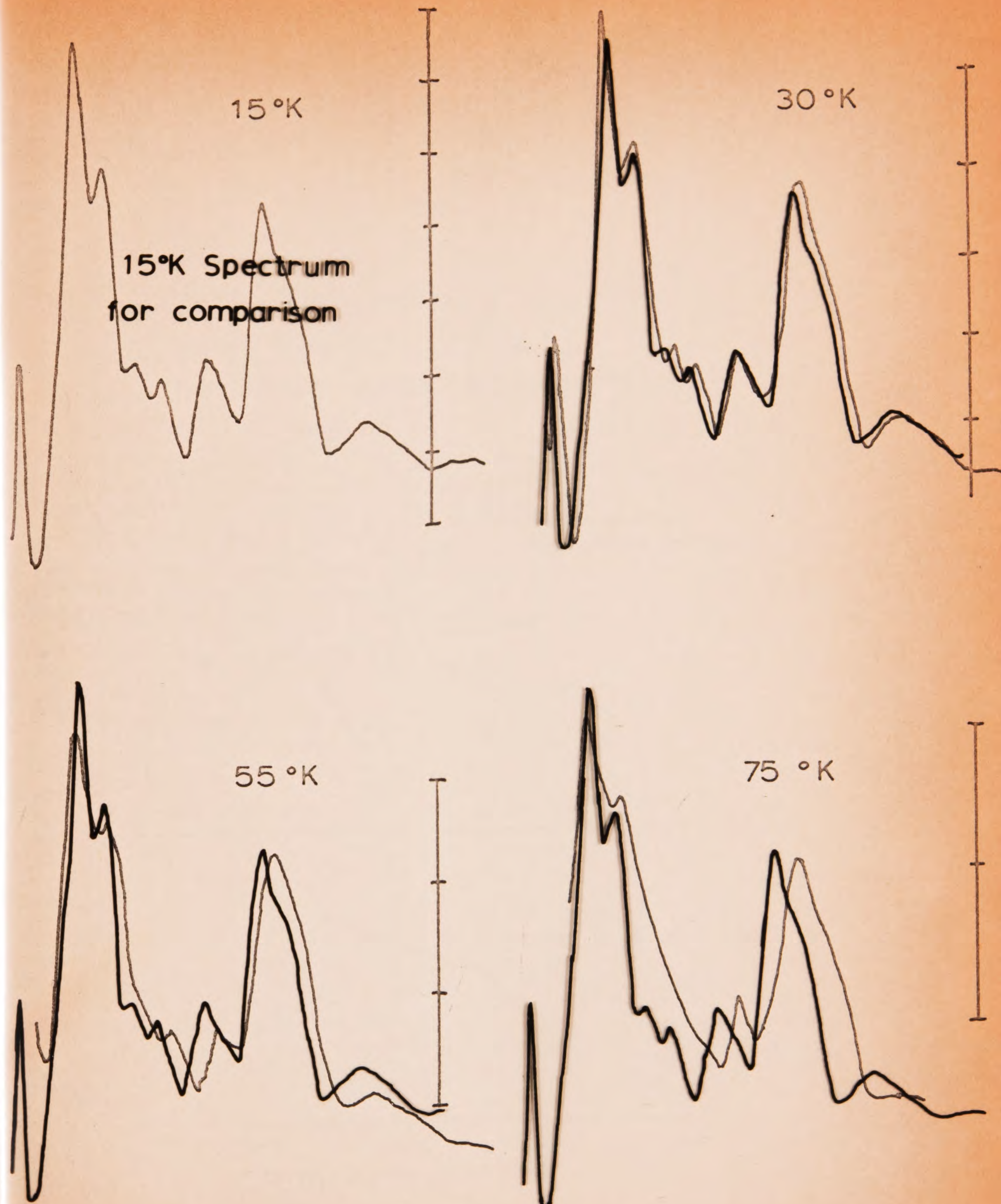
Figure 6·16 Band Shape Fitting Ni^{++}-ZnO Sigma



Ni^{++}-ZnO E⊥C

One scale division
= 0·05 Absorbance

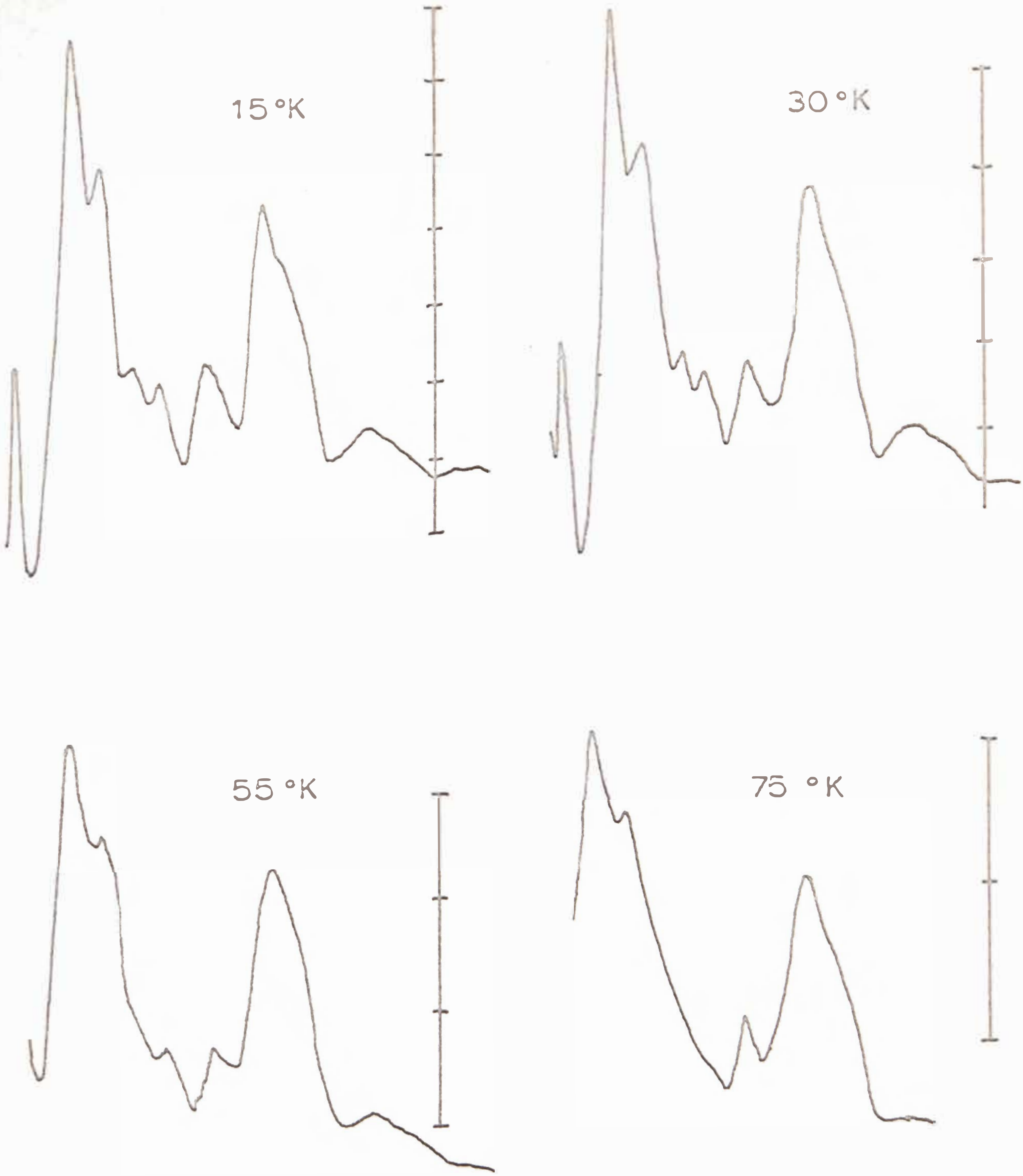
Figure 6·17 Ni^{++}-ZnO Pi Band Shape Fitting



Ni^{++}-ZnO
E //C

One scale division
= 0·05 Absorbance

Figure 6·17 Ni^{++}-ZnO Pi Band Shape Fitting



Ni^{++}-ZnO
E //C

One scale division
= 0·05 Absorbance

Figure 6·18 Temperature Dependence of Weak Line Areas (J–A)
(For the whole weak structure)

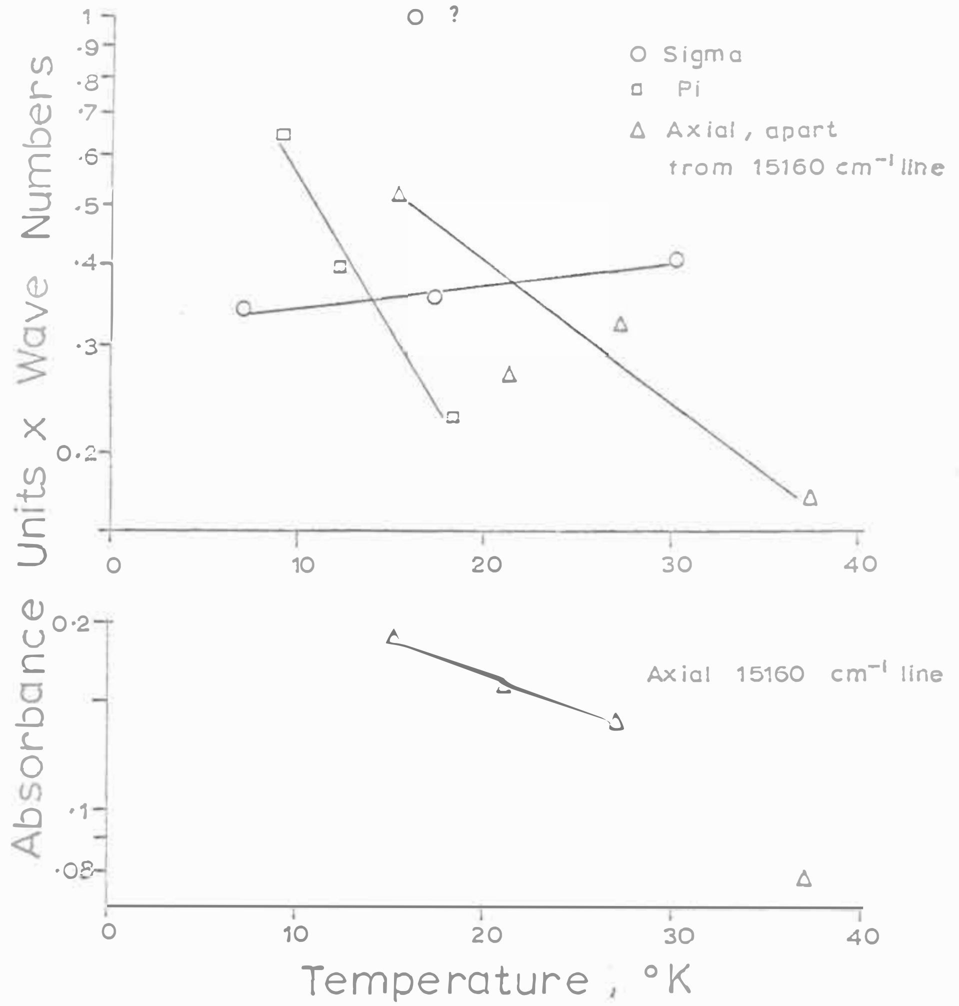


Figure 7-1 d^8 Under Decreasing Perturbations

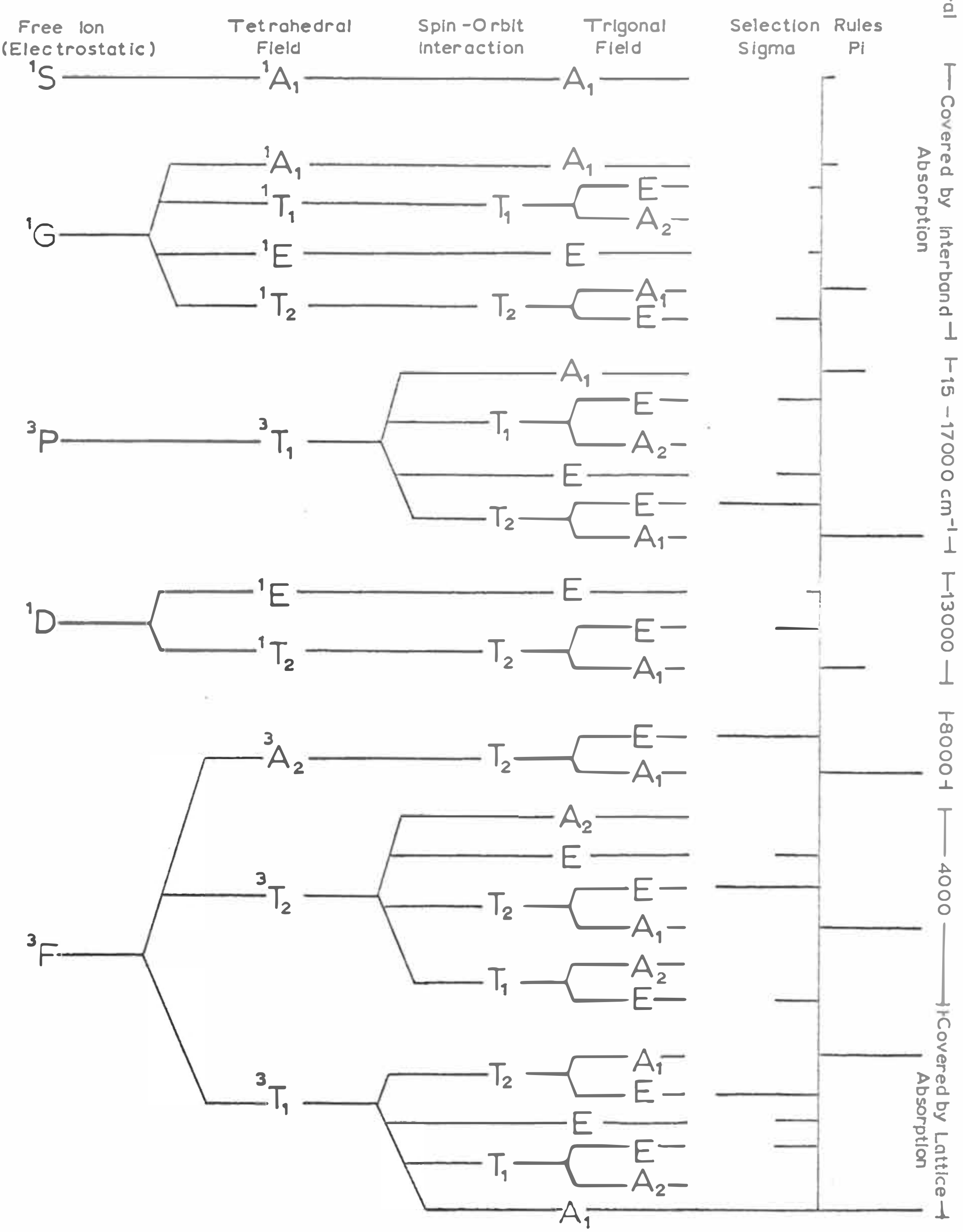


Figure 7·2 Pairs in Ni-ZnO

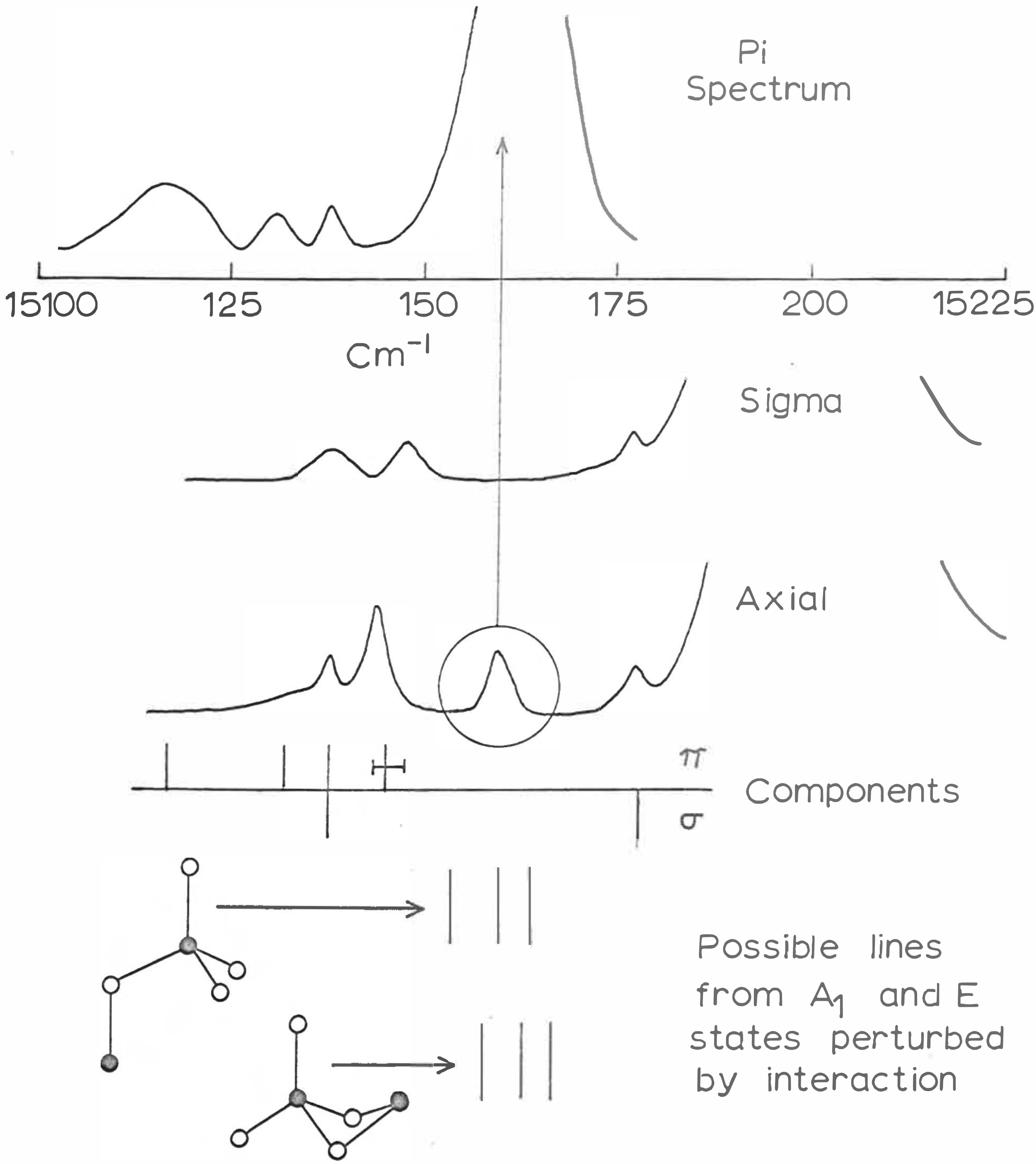
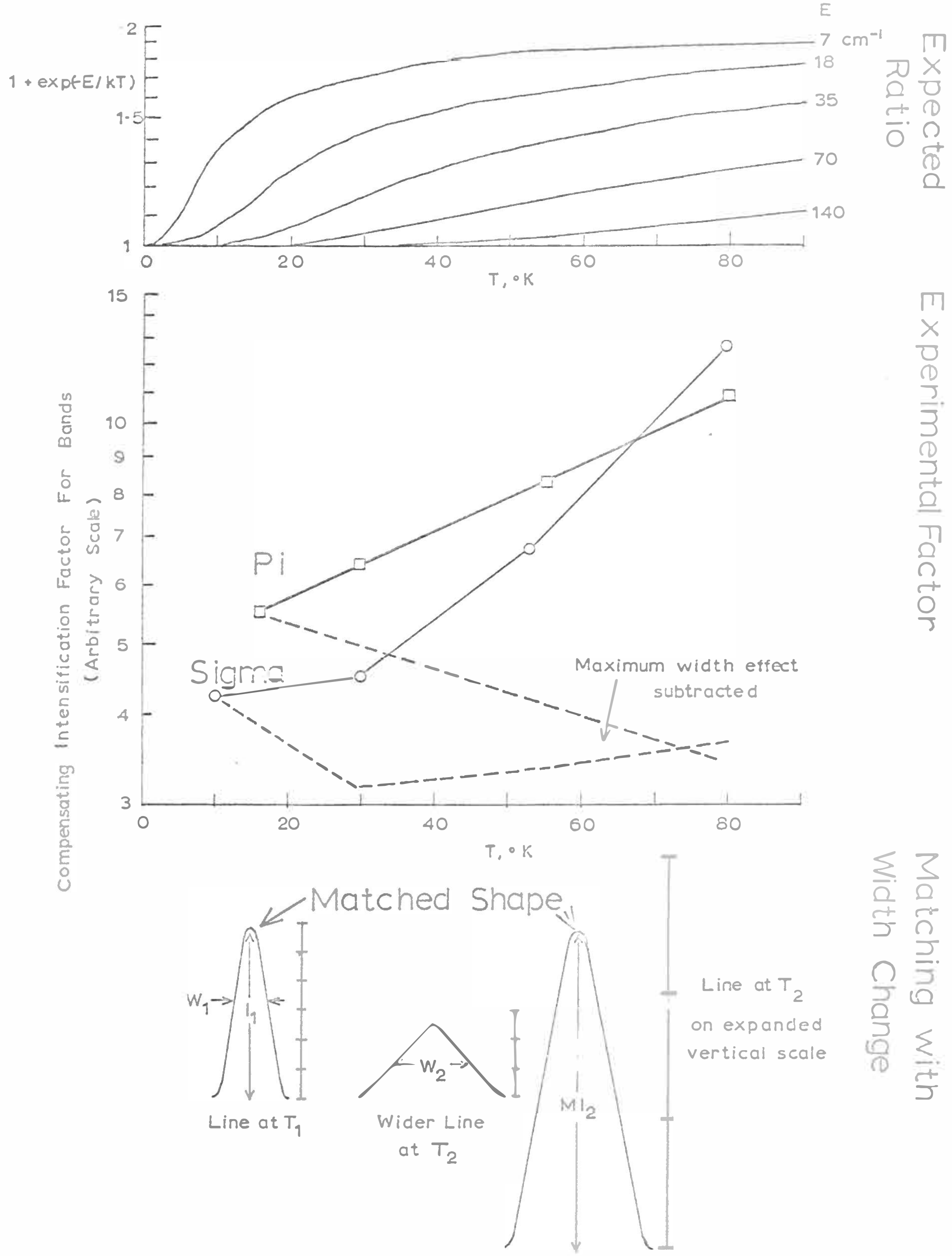


Figure 7·3 d^2 Cubic Field

Trigonal and cubic field representations and the main multiplet component are given for each level. The first line gives parameter values, the body of the table gives parameter dependence.

ENERGY	STATE				A40	A43	A20	DELTA	V	VPRIME	ZETA	B	C
					-7027.944	8400.000	0.000	4199.99	0.00	0.00	-500.	770.	3700.
47024	A1		1	S	-.0497	.1190	0.0000	.321	0.000	0.000	-.18846	13.73065	6.86017
22942	E		1	G	-.1582	.3783	0.0000	1.021	0.000	0.000	-.14961	2.04830	1.99317
21128	A1		1	G	-.0123	.0294	0.0000	.079	0.000	0.000	-.06443	4.25256	2.12524
20958	A2	T_1	1	G	-.1193	0.0000	.1194	.199	-.332	0.000	-.05134	3.99181	1.99855
20958	E		1	G	.0132	.1109	-.0597	.199	.166	0.000	-.05135	3.99181	1.99855
19356	A1	T_2	1	G	-.0888	-.0854	-.0740	-.022	-.109	-.671	-.13803	3.10199	1.99102
19356	E		1	G	.0495	.0303	.0370	-.022	.054	.335	-.13803	3.10199	1.99102
15646	A1		3	P	-.0120	.0287	0.0000	.077	0.000	0.000	-.76688	6.83448	.01327
15454	A2	T_1	3	P	-.0066	.0352	-.1428	.081	.183	-.455	-.48399	6.81091	.00012
15454	E		3	P	-.0156	.0277	.0714	.081	-.091	.227	-.48399	6.81092	.00012
15251	E		3	P	.0047	-.0114	0.0000	-.030	0.000	0.000	-.56330	5.60024	.31424
15148	A1	T_2	3	P	.0106	.0176	.1214	.017	-.116	.471	-.21746	6.13035	.16784
15148	E		3	P	-.0093	.0008	-.0607	.017	.058	-.235	-.21746	6.13035	.16784
13330	E		1	D	.0783	-.1872	0.0000	-.505	0.000	0.000	.97656	.10986	1.68455
12873	A1	T_2	1	D	.2311	-.0534	-.0277	-.493	.365	.612	.38863	-1.54714	1.81299
12873	E		1	D	-.0008	-.2475	.0138	-.493	-.182	-.306	.38863	-1.54714	1.81299
8582	A1	T_2	3	F	-.1769	.4344	.0023	1.164	.004	.024	-.27505	-7.95999	.01506
8582	E		3	F	-.1822	.4299	-.0011	1.164	-.002	-.012	-.27505	-7.95999	.01506
4555	A2		3	F	-.0309	.0740	0.0000	.199	0.000	0.000	-.50000	-8.00000	0.00000
4361	E		3	F	-.0229	.0549	0.0000	.148	0.000	0.000	-.47018	-7.96999	.00429
4331	E	T_2	3	F	-.0449	.0643	.0321	.203	-.067	.047	.13208	-7.95369	.01086
4331	A1		3	F	-.0048	.0978	-.0643	.203	.134	-.095	.13209	-7.95369	.01086
4235	E	T_1	3	F	-.0004	.0924	-.0248	.185	.090	.045	.03470	-7.99186	.00046
4235	A2		3	F	-.0853	.0214	.0497	.185	-.181	-.090	.03470	-7.99186	.00046
1028	E	T_2	3	F	.1569	-.2039	-.0211	-.670	.139	.170	-.39016	-7.77149	.00219
1028	A1		3	F	-.0021	-.3370	.0423	-.670	-.278	-.340	-.39016	-7.77149	.00219
878	E		3	F	.0981	-.2345	0.0000	-.633	0.000	0.000	.20654	-7.78842	.00371
311	E	T_1	3	F	.0338	-.3052	.0131	-.667	-.165	-.272	1.00064	-7.81086	.00086
311	A2		3	F	.2423	-.1308	-.0263	-.667	.330	.545	1.00064	-7.81087	.00085
0	A1		3	F	.1051	-.2513	0.0000	-.678	0.000	0.000	1.51978	-7.81769	.00130

Figure 7-4 Depopulation and Band Intensity



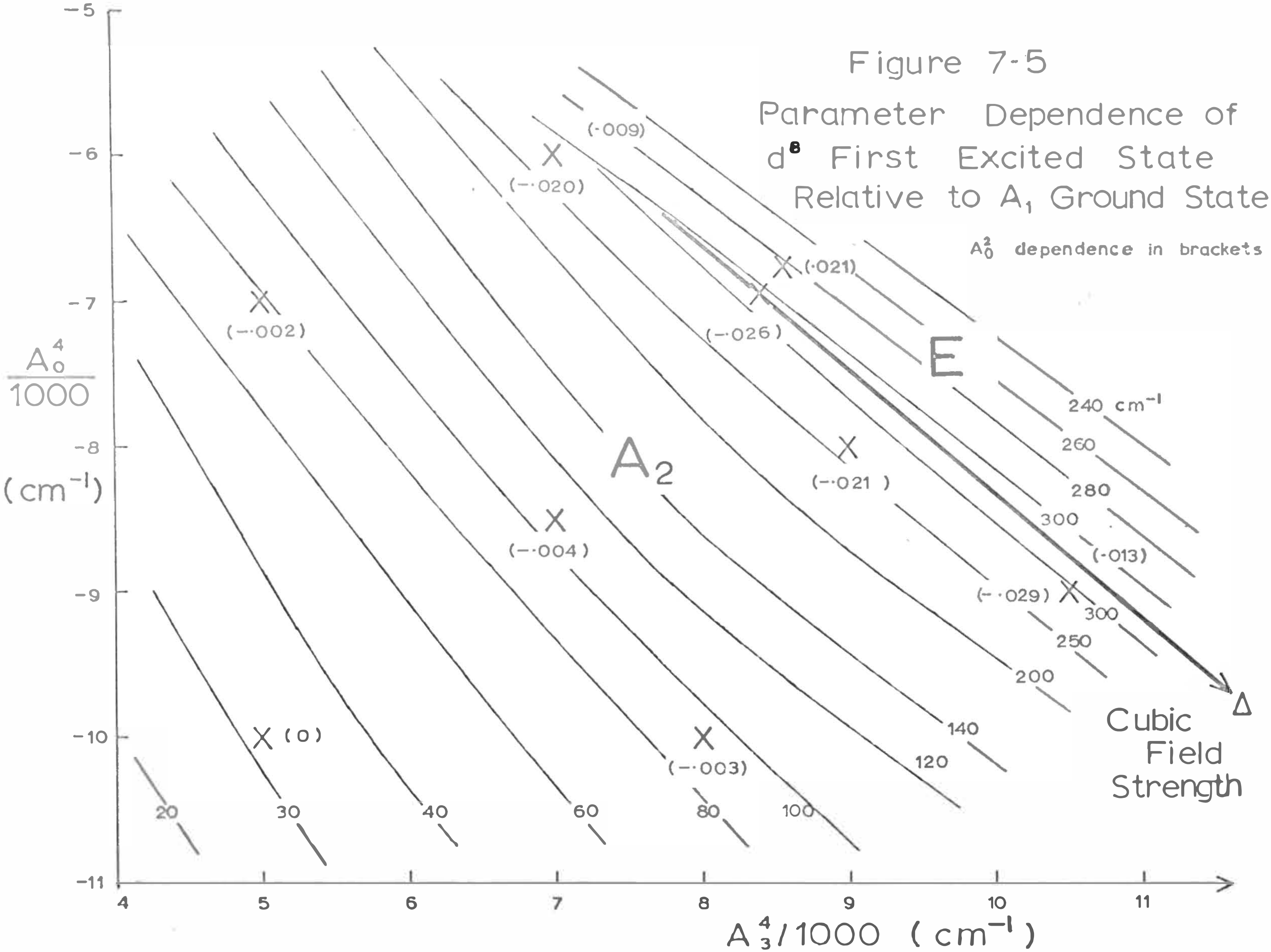


Figure 7-5
Parameter Dependence of
d⁸ First Excited State
Relative to A₁ Ground State
A²₀ dependence in brackets
A⁴₀/1000
(cm⁻¹)
A⁴₃/1000 (cm⁻¹)
-5
-6
-7
-8
-9
-10
-11
4
5
6
7
8
9
10
11
A₂
E
(·009)
(-·020)
(·021)
(-·026)
(-·002)
(-·021)
(-·004)
(·013)
(-·029)
(0)
(-·003)
240 cm⁻¹
260
280
300
300
250
200
140
120
100
80
60
40
30
20
Cubic
Field
Strength
Δ

Figure 7·6 V and V′ Dependence of Splittings

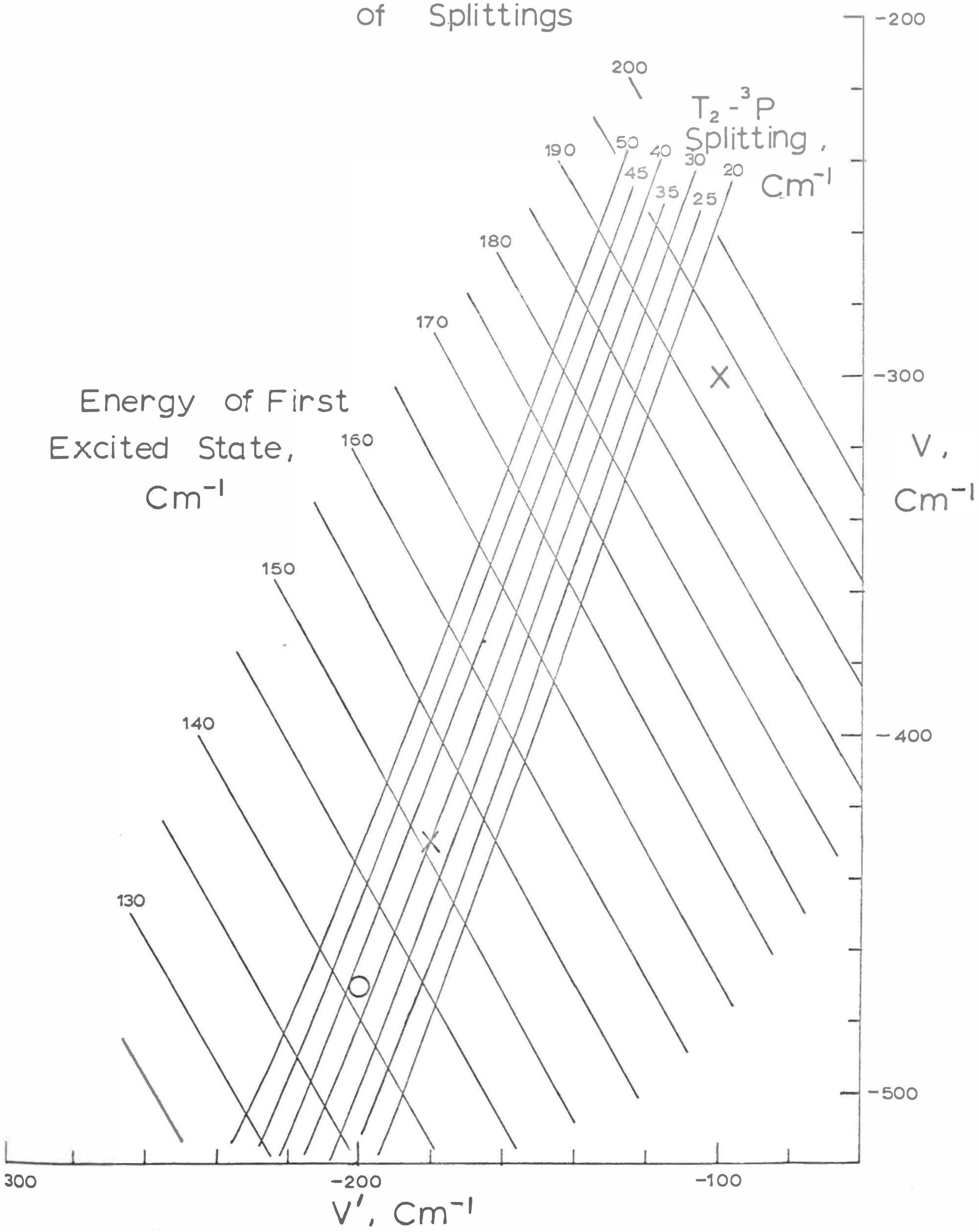


Figure 7-7 Trigonal Field Levels

Parameters are chosen to fit the energies of the first excited state and the two components of T_2 (^3P)

ENERGY	STATE		DELTA	V	VPRIME	ZETA	B	C	Energy for	No-Phonon Lines
			4199.99	-469.99	-199.99	-500.	770.	3700.	B = 765.5	
47136	A1	1 S	.291	-.014	-.052	-.19069	13.77263	6.88109	47039	
23079	E	1 G	1.010	-.001	-.329	-.14817	2.06364	1.99328	23035	
21255	A1	1 G	.108	-.035	.005	-.06158	4.20062	2.09951	21201	
21218	A2	1 G	.199	-.332	0.000	-.05021	3.99214	1.99862	21165	
20962	E	1 G	.206	.109	.161	-.05422	3.95731	1.99835	20929	
19628	A1	1 G	-.008	-.060	-.606	-.13879	3.02790	1.99590	19579	
19354	E	1 G	-.028	.037	.360	-.13788	3.15434	1.99070	19304	
15756	A1	3 P	.078	-.003	-.047	-.76582	6.82460	.01330	15689	
15566	A2	3 P	.078	.169	-.453	-.48722	6.82210	.00009	15499	
15563	E	3 P	.084	-.099	.173	-.48115	6.78785	.00020	15496	
15381	E	3 P	-.041	-.128	.035	-.61843	5.42727	.34698	15321	
15264	E	3 P	.012	.148	-.367	-.24377	6.11033	.17603	15201	15200
15226	A1	3 P	.040	-.137	.384	-.08828	6.29705	.12070	15163	15163
13543	E	1 D	-.473	-.301	-.265	.99514	-.00418	1.65115	13540	
12992	E	1 D	-.502	.163	.098	.47126	-1.27521	1.80760	12989	
12668	A1	1 D	-.519	.439	.590	.20739	-1.70527	1.85488	12665	
8680	E	3 F	1.163	-.002	.085	-.29032	-7.94286	.01373	8680	
8669	A1	3 F	1.159	.004	.124	-.23913	-7.91115	.01885	8669	8343
4694	A2	3 F	.199	-.157	.003	-.42280	-7.99891	.00006	4694	
4598	E	3 F	.170	-.322	-.043	-.19270	-7.95787	.00696	4598	
4414	A2	3 F	.178	-.024	-.159	-.07374	-7.98178	.00036	4414	
4399	A1	3 F	.188	.130	-.160	.06252	-7.93376	.01237	4399	
4375	E	3 F	.180	.152	-.043	-.11131	-7.96224	.00701	4375	4248
4259	E	3 F	.186	.177	0.000	.05077	-7.98741	.00107	4259	4217
1421	A1	3 F	-.667	-.485	-.628	-.19040	-7.74327	.00206	1421	
1295	E	3 F	-.650	-.477	-.601	.16492	-7.75657	.00276	1295	
863	E	3 F	-.657	.281	.382	-.19665	-7.79601	.00275	863	
372	E	3 F	-.661	.212	.332	.79253	-7.81839	.00134	372	
141	A2	3 F	-.656	.345	.607	1.03399	-7.63355	.00084	141	(140)
0	A1	3 F	-.671	.222	.390	1.40480	-7.82934	.00128	0	

Figure 7-8 Wurtzite $\underline{k} = \underline{0}$ Modes

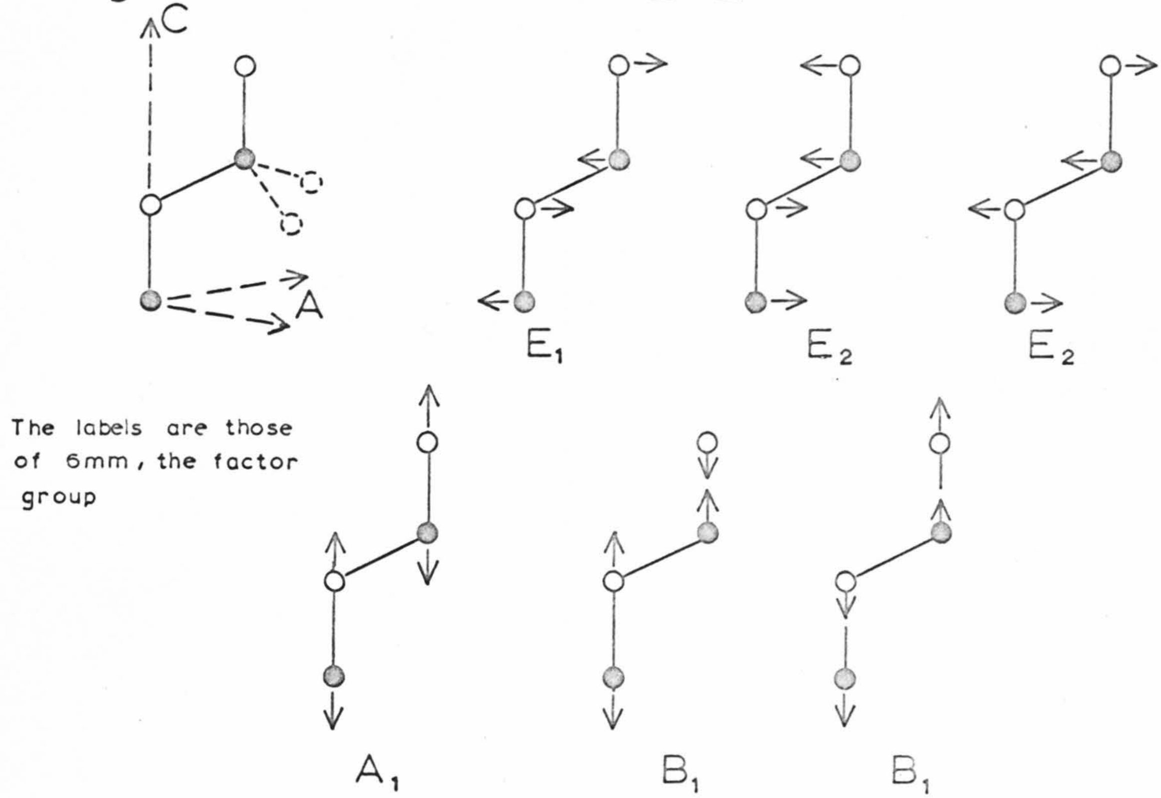


Figure 7-9 Peaks in the ZnO Phonon Distribution

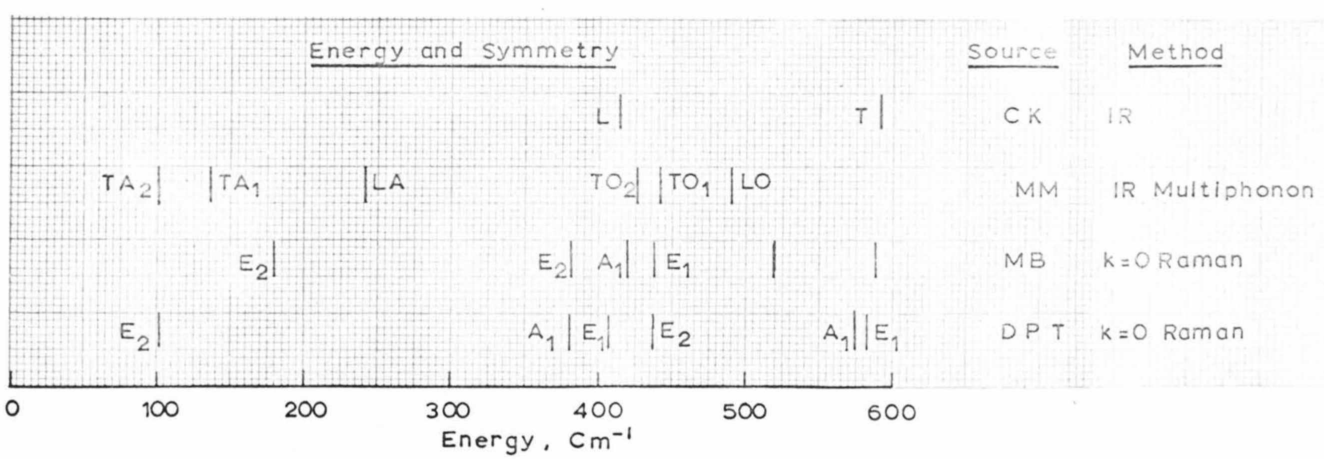
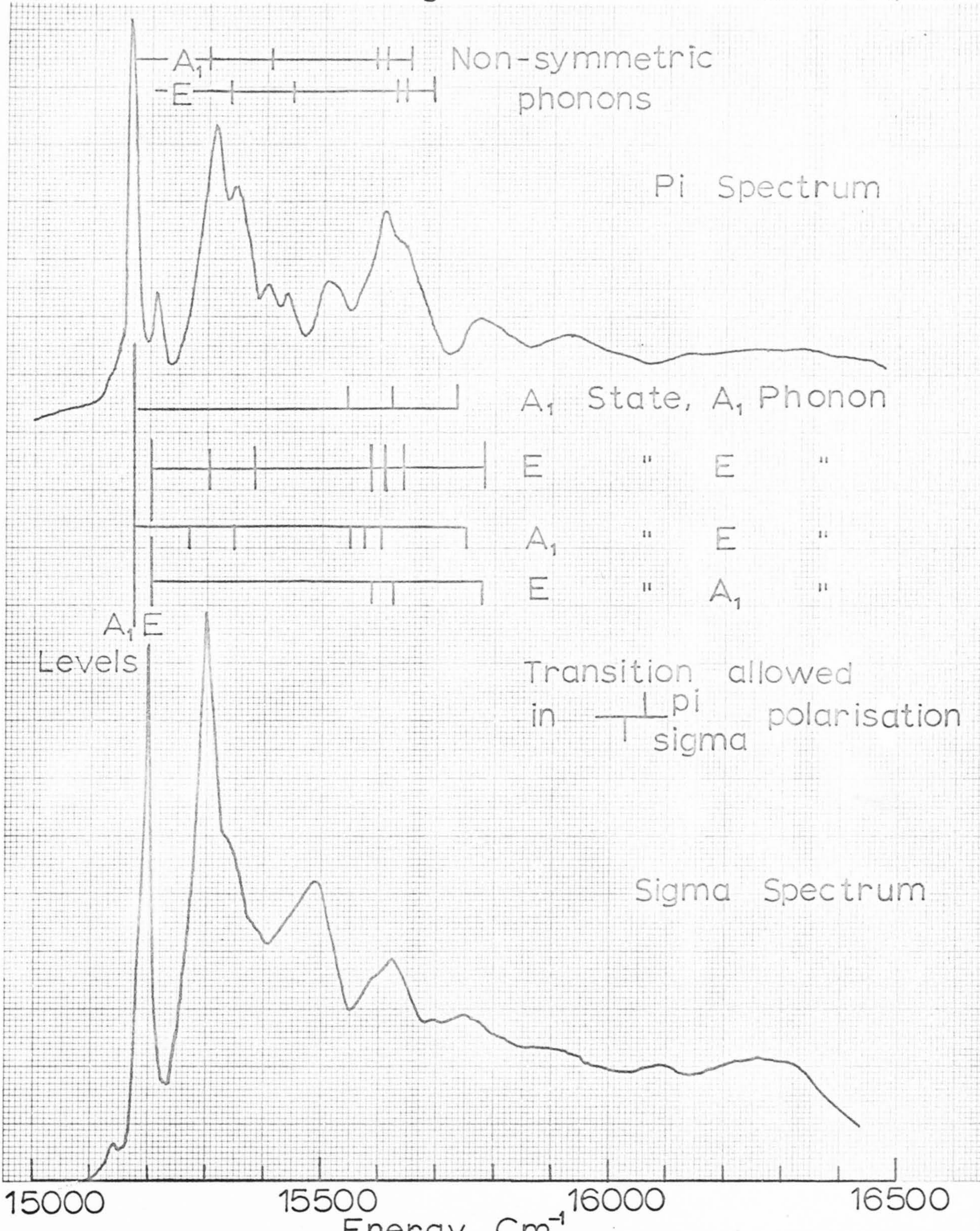


Figure 7-10 Phonon Fitting for the Ni-ZnO Visible Bands



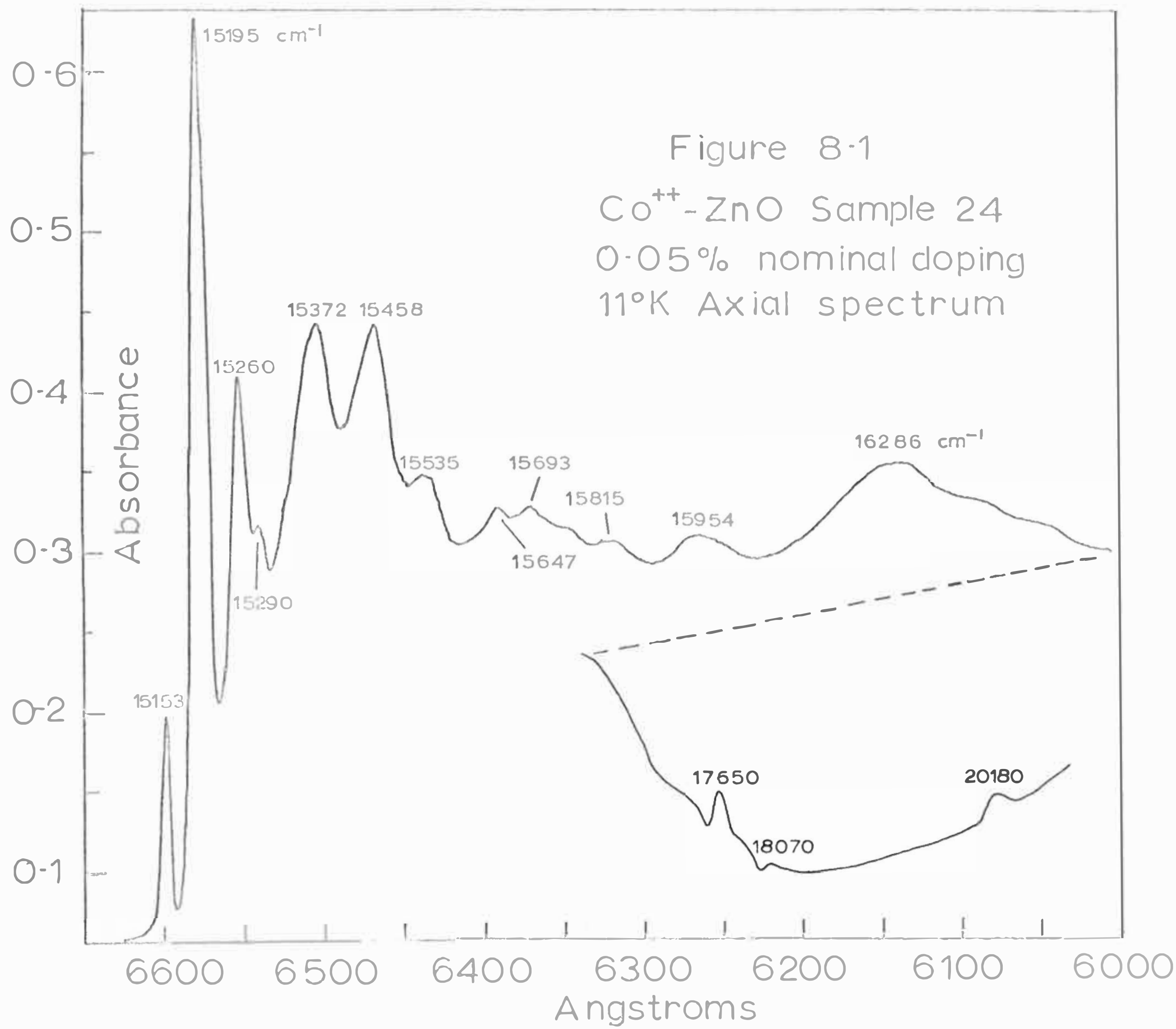
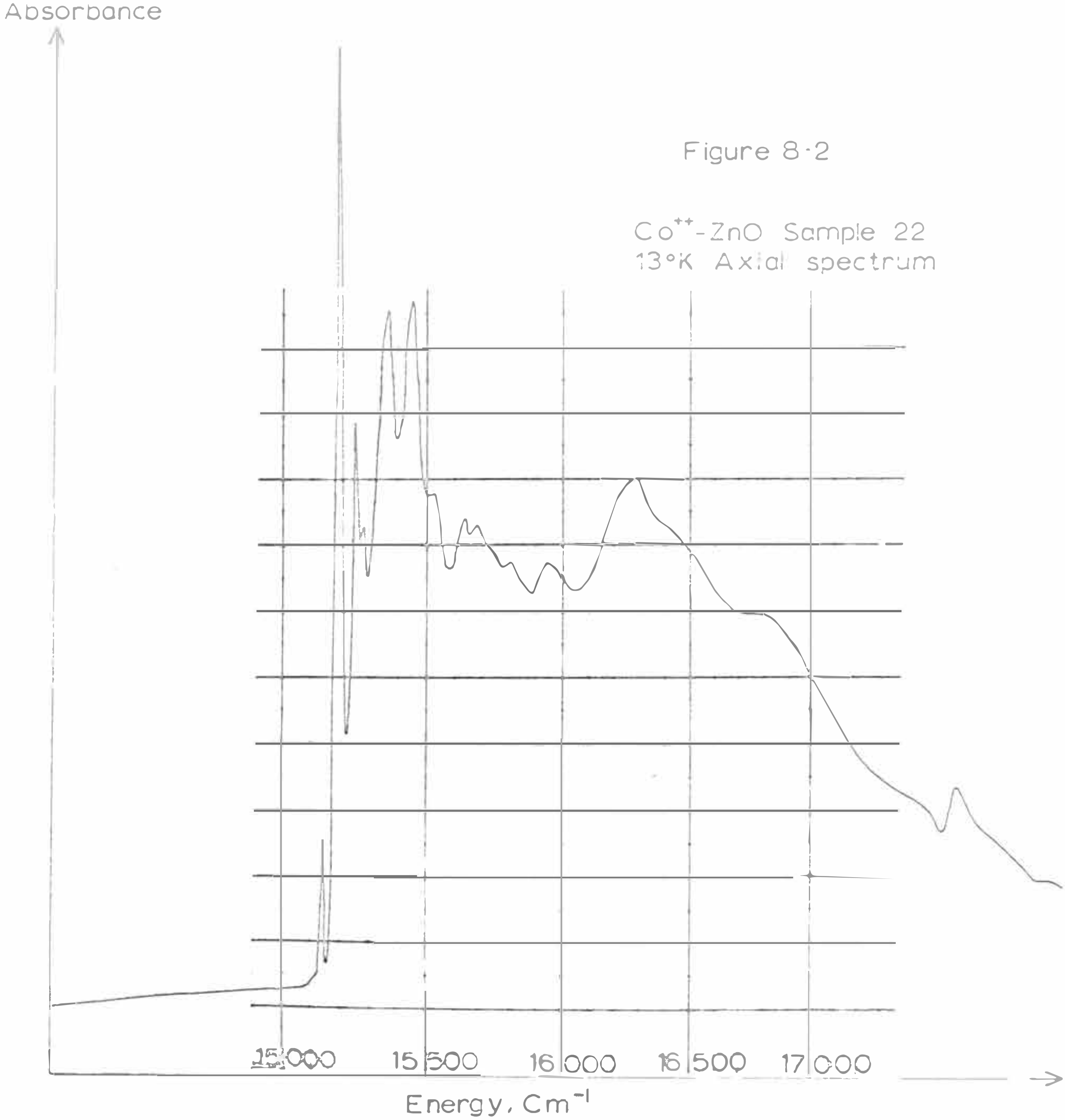


Figure 8·1
Co++-ZnO Sample 24
0·05% nominal doping
11°K Axial spectrum
Absorbance
Angstroms
0·1
0·2
0·3
0·4
0·5
0·6
6600
6500
6400
6300
6200
6100
6000
15195 cm-1
15153
15260
15290
15372
15458
15535
15647
15693
15815
15954
16286 cm-1
17650
18070
20180


Absorbance
Figure 8-2
Co++-ZnO Sample 22
13°K Axial spectrum
15000
15500
16000
16500
17000
Energy, Cm-1

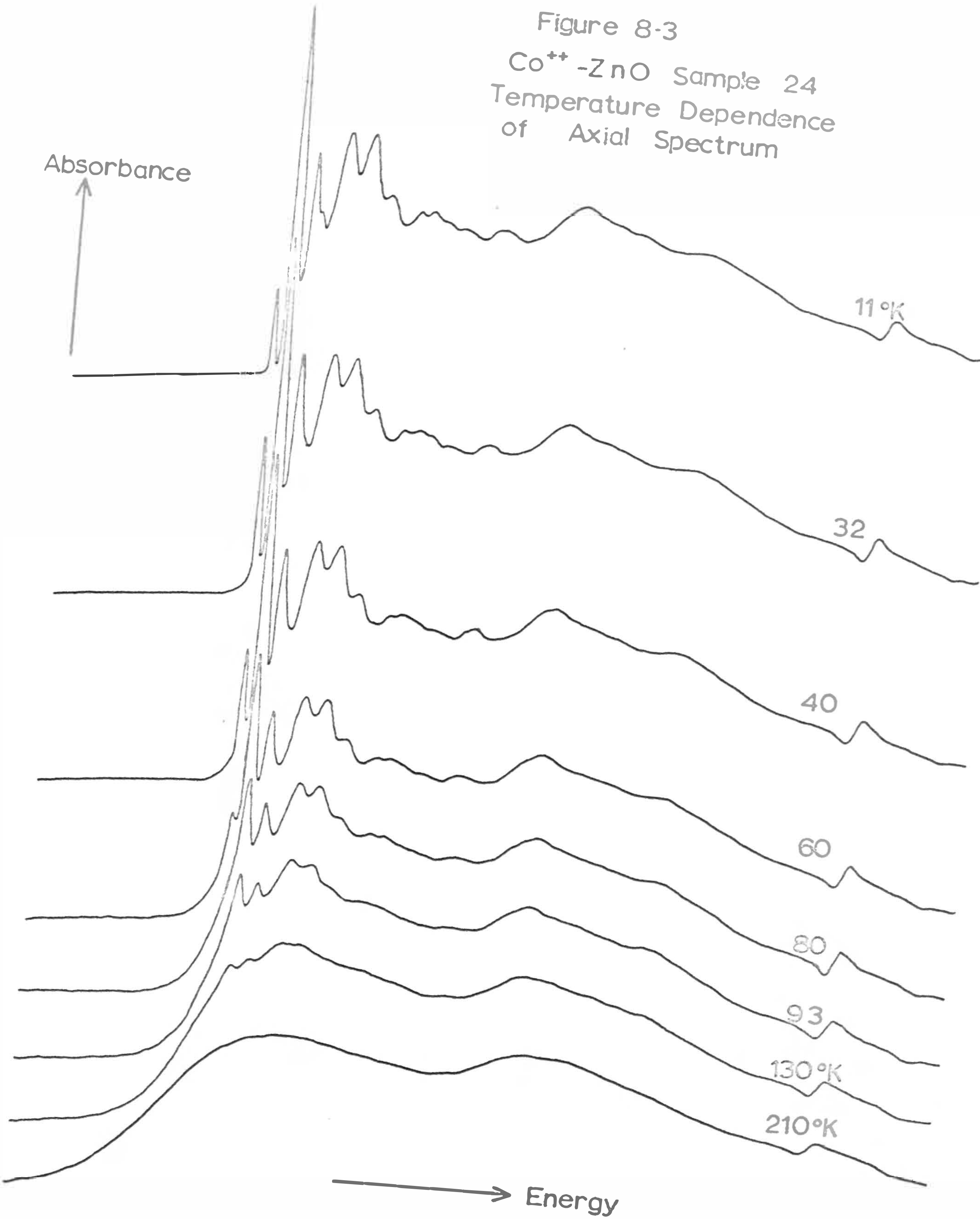


Figure 8-3
Co^{++}-ZnO Sample 24
Temperature Dependence
of Axial Spectrum
Absorbance
Energy
11 °K
32
40
60
80
93
130 °K
210 °K

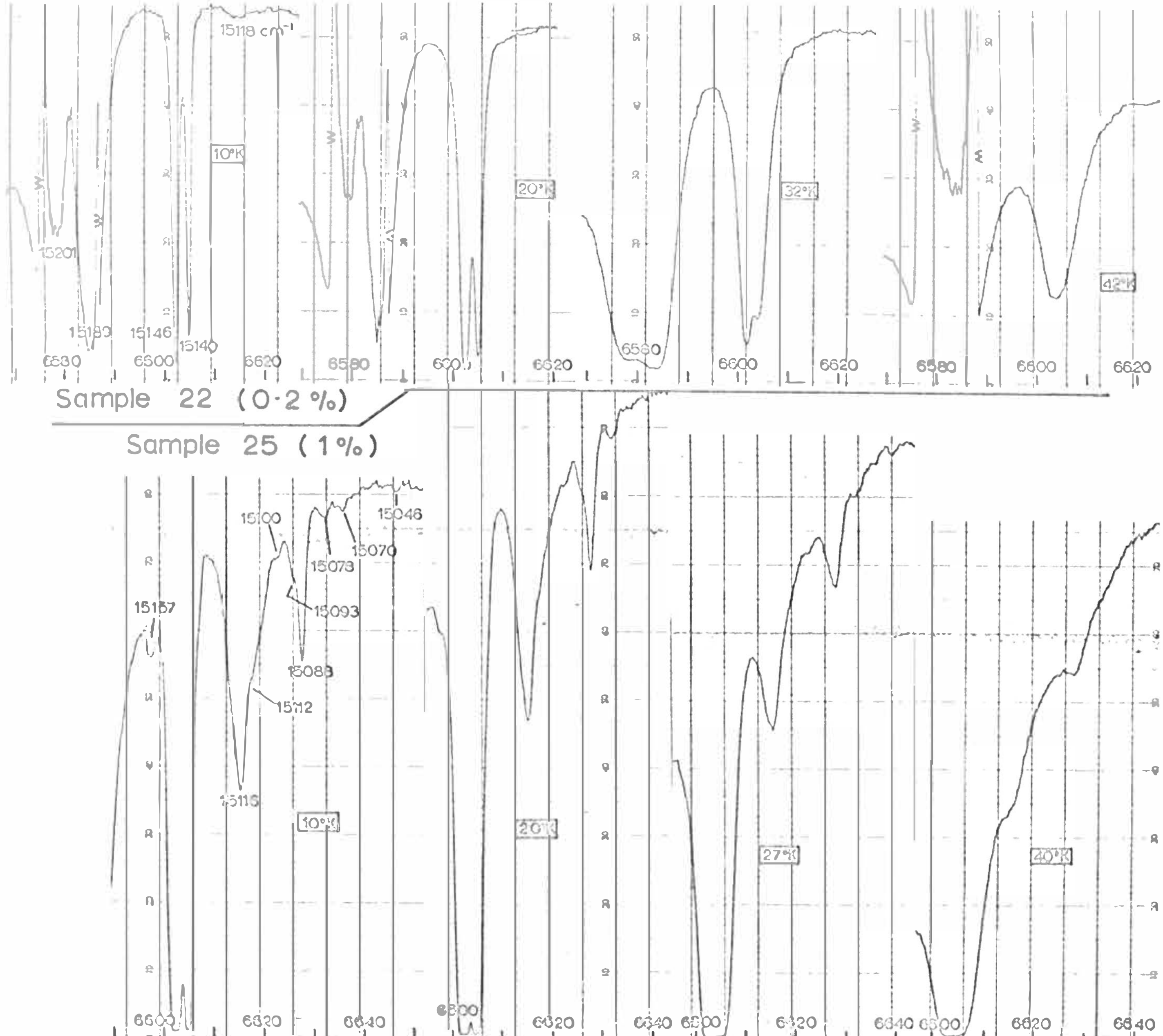


Figure 8·4 Co^{++}-ZnO Axial Spectrum (J-A)

Figure 8-5 Co^{++}-ZnO Pi Spectrum (J-A)

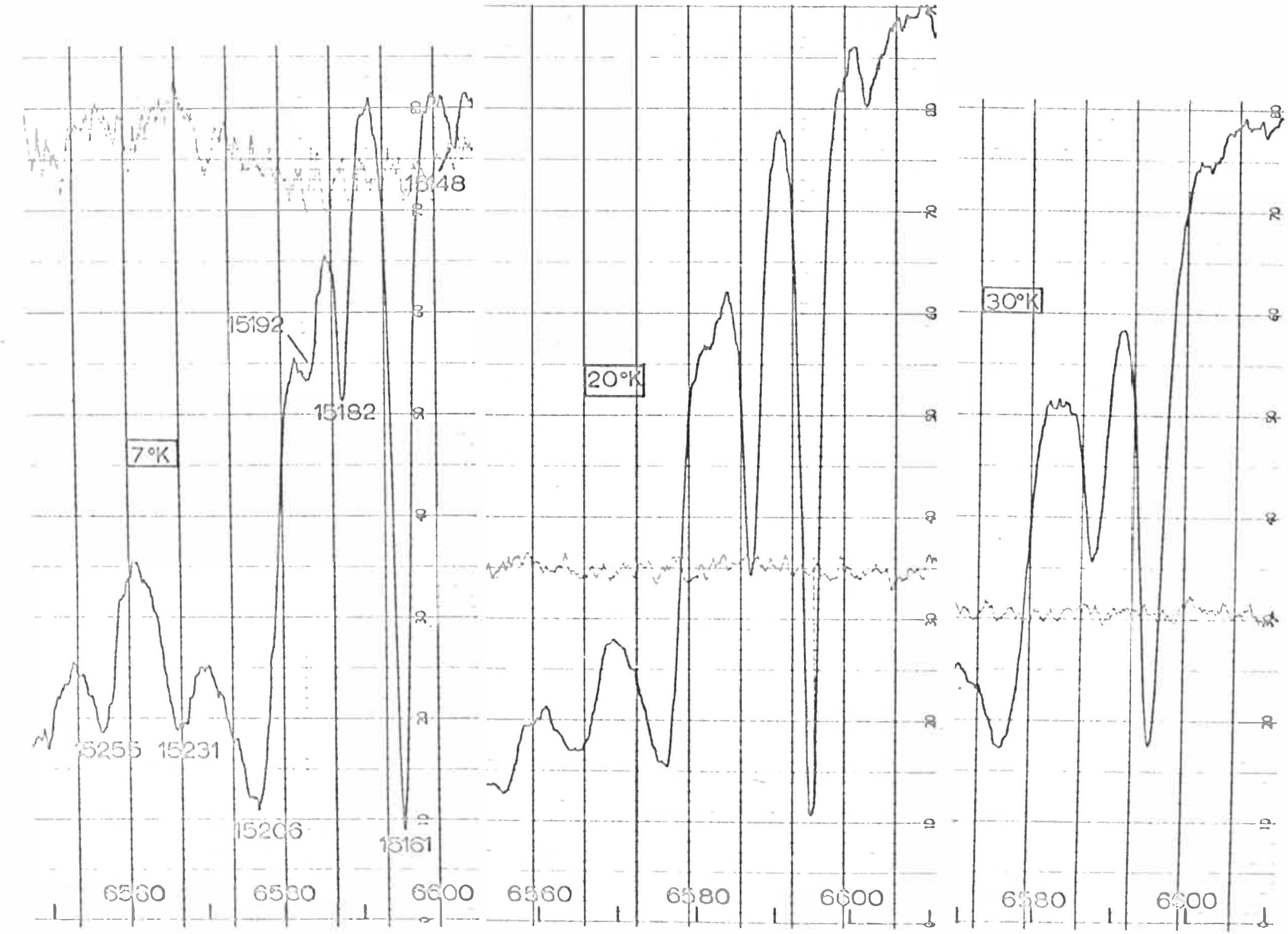


Figure 8-6 Concentration Dependence of Co-ZnO Weak Lines

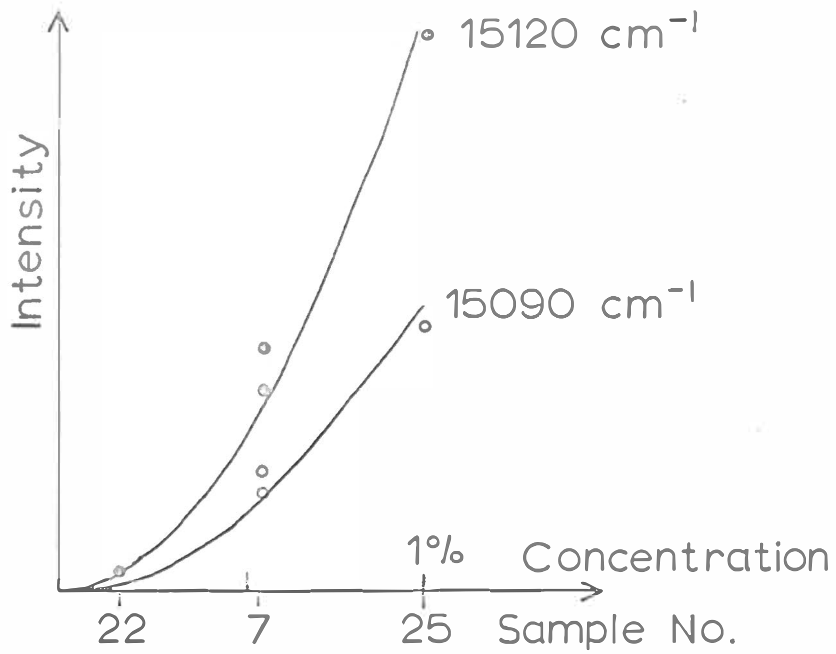
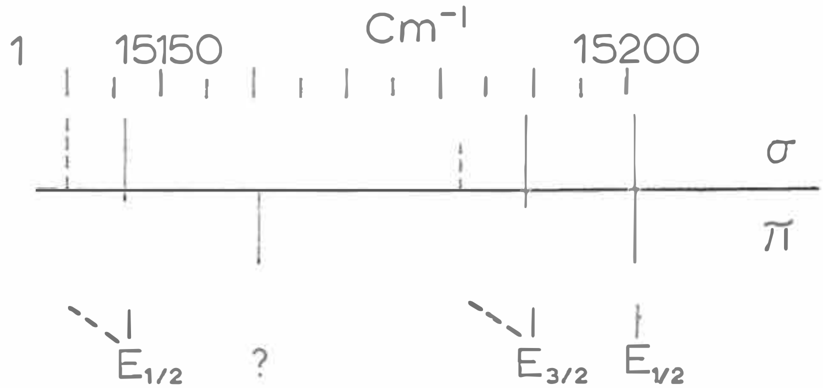


Figure 8-7 The No-Phonon Lines



Dotted Lines show thermal populating

Figure 8-8 Phonon Fitting for the Co-ZnO Axial Spectrum

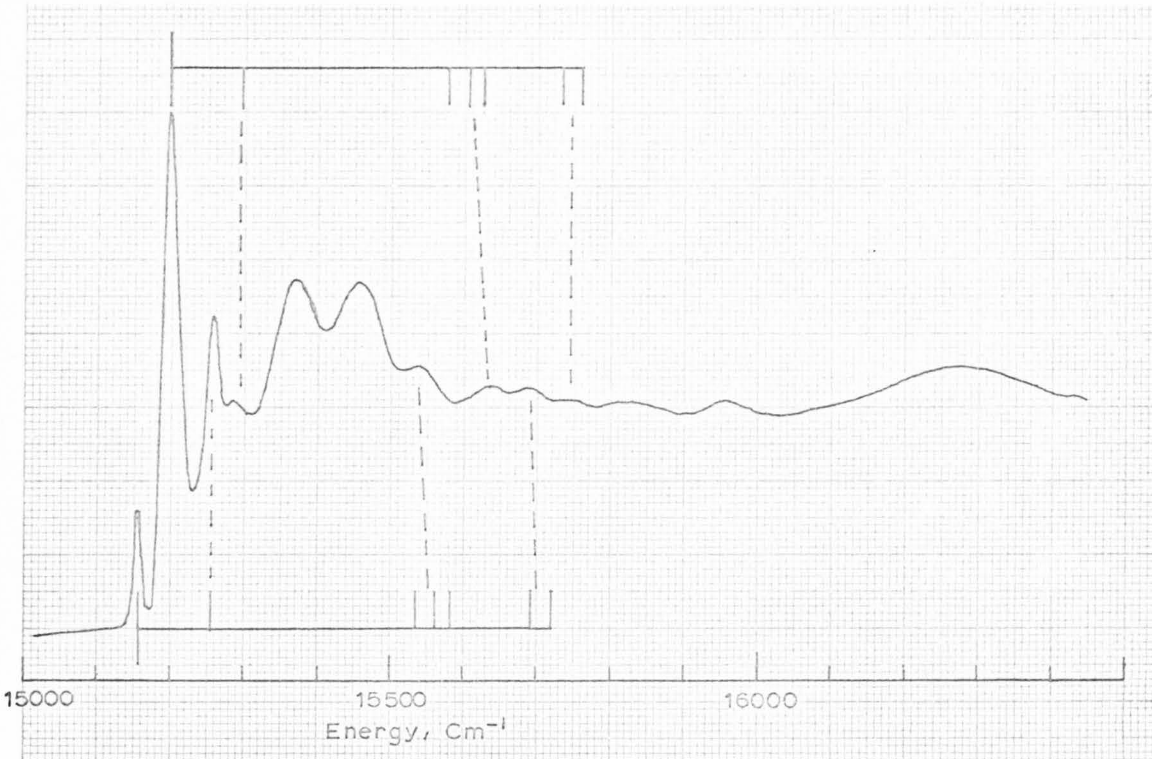
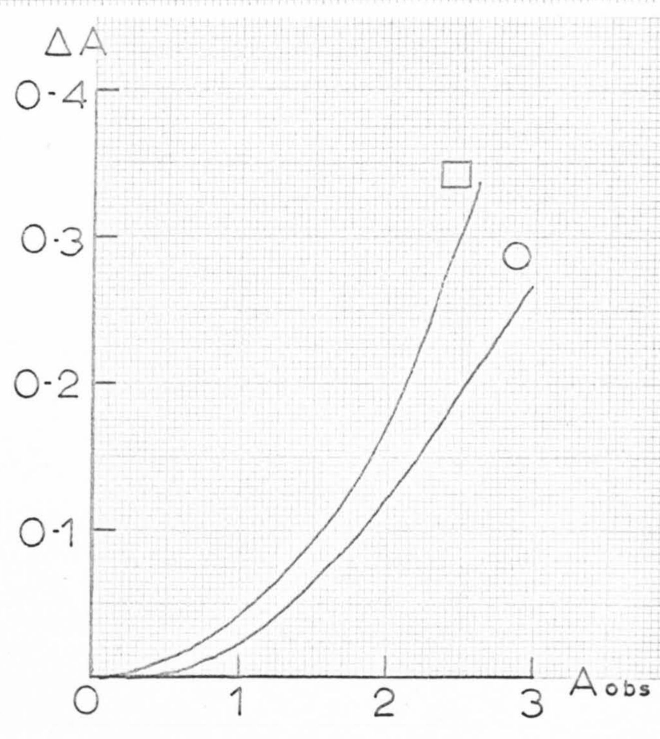


Figure A1

Correction to Apparent Absorbance for a Crystal Wedge



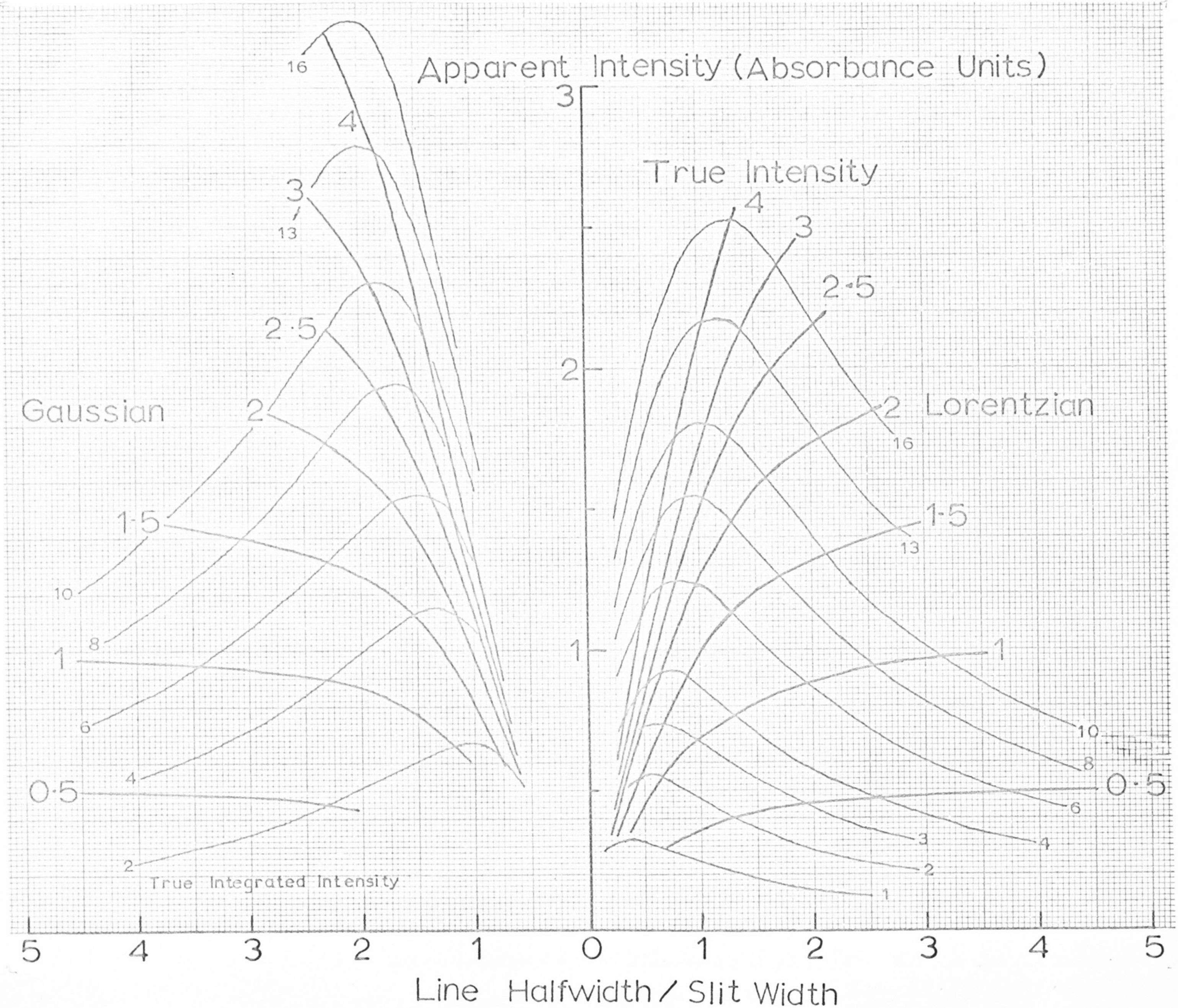


Figure A2 Apparent Intensity of Slit-limited Absorption Lines as a Function of Width

APPENDIX ONE

HEAT FLOW IN THE SAMPLE HOLDER AND SAMPLE

The heat input to the sample holder will be from two sources.

1 Black body radiation from the nitrogen shield and through the windows.

2 Energy absorbed from the light beam.

For both, take a worst possible case.

1 The nitrogen shield had two windows of $3\ cm^2$ area. Assume that all the radiation from a black body at $300^{o}K$ passing through these windows is absorbed by the holder. Then heat flow in

$$W = A\,\sigma\,T^4$$

$$= 6 \times 5.7 \times 10^{-12} \times 300^4 \text{ watts}$$

$$= 0.28 \text{ watts.}$$

The holders were electropolished, giving an emissivity[62] of say 0.02, so this can be reduced to 6 mw.

2 The lamp filament is imaged onto the crystal by the condenser system. For a final image 2 mm high produced by rays in 0.6 sterad of solid angle, 0.3% of the light from an 8 mm filament is used. Assuming the lamp is 1% efficient, radiating 1 watt of visible light, 3 mw is incident on the sample. This is less than the previous power, and so does not affect the sample holder, but being incident directly on the crystal, which has low thermal conductivity, it may raise its temperature above that of the

holder.

Now assuming a 1 cm path length between crystal and dewar base, with heat flow across a 0.2 cm^2 area, we have

$$W = k\ A\ \frac{\Delta T}{l}$$

$$\Delta T = \frac{W}{k}\frac{l}{A}$$

Taking k = 1 watt/cm deg K at 10 degrees, for commercial copper,

ΔT = 1.5 degrees K for 0.3 watts.

The lowest temperature actually observed was $7^{\circ}K$, i.e. $\Delta T = 2.8$ degrees. The extra could have occurred across the Indium gasket or be due to poor thermocouple contact.

For temperature gradients across the crystal, consider 3 mw flowing from a line image in the crystal, through an area of typically 1 mm^2, for 1 mm distance. Then from $\Delta T = Wl/(kA)$, we have $\Delta T = \frac{3}{100k}$, with T in degrees and k in watts/cm $^{\circ}K$. Since k will certainly be higher than 0.01, ΔT will be less than $3^{\circ}K$, and may be much less. The actual differential will of course vary with sample and sample mounting.

APPENDIX TWO

ABSORBANCE OF A WEDGE-SHAPED CRYSTAL

Consider a homogeneous beam of monochromatic light of intensity I incident on an area of crystal for which the thickness is a linear function of one co-ordinate x, with the origin as the crystal centre,

$$t = ax + t_o,$$

and optical density α.

Then light transmitted

$$= I\int e^{-\alpha t(x,y)}\,dxdy$$

$$= I\ A\ e^{-\alpha t_o}\ K,$$ where A is the area observed and K depends on a, α, and the geometry. If A is a rectangular area aligned to the axes, and of x dimension 2d,

$$K = \frac{\sinh(\alpha ad)}{2\alpha ad}.$$

If A is a circular area of radius r, the result is

$$K = \frac{2\ I_1(\alpha ad)}{\alpha ad}$$

where I_1 is the modified Bessel function of the first kind, of first order.

The correction appropriate absorbance is ln(K).

Figure A1 shows this as a function of apparent absorbance for parameters appropriate to sample 6.3 and its holder and the correction for a square hole of the same diameter.

APPENDIX THREE

INSTRUMENTAL EFFECTS IN SPECTRA

The two effects observed in the spectra of Chapter Six, namely slit limiting on the Bausch and Lomb and intensity cutoff on the Jarrell-Ash, will be discussed here.

Intensity Limiting of Absorption Lines

The spectra showed a cutoff of intensity at absorbance 2 which could not be accounted for by errors in the zero level, and was below the expected noise limit. The limiting must therefore have been caused by stray light passing the crystal by some means and reaching the detector.

Polarised light was used, and since the two strong lines observed were at different wavelengths, any light of incorrect polarisation would be passed by the crystal. The expected transmittances were 0.06% due to polarisation impurity and 0.2% for incorrect alignment. Transmittances are additive to give the final intensity reaching the detector.

It was found that due to an internal reflection in the quartz plate in the Jarrell-Ash used to direct energy to the monitor phototube, a ghost spectrum was formed at the exit slit displaced 1 mm from the main spectrum. With dispersion 3.3 A/mm, this was sufficient to partially clear the strong lines and give a transmittance estimated at 0.2% at the line peaks.

The three contributions add to give transmittance 0.5%, corresponding to absorbance 2.3, which is near the observed limit. Some of the errors may be underestimated, or other effects may be significant. McClure[31] found that accurate readings were only obtained after small cracks in the crystals were filled to stop residual transmission.

Slit-Limiting of Absorption Lines

The calculations of Kostkowski and Bass[32] do not cover many cases, and Kyle and Green[33] give figures only for the transmittance and halfwidth of Lorentzian lines. It was decided to perform similar calculations for Gaussian and Lorentzian lines for results in absorbance units. The slit function was taken as Gaussian for convenience.

The integrations to find apparent line intensity were done for lines of constant true integrated area and varying width, using a computer program. From the plots of the results, curves showing apparent intensity as a function of width for lines of constant real intensity can also be drawn, as in Figure A2. The curves of constant integrated intensity are of interest to the present spectra, since no-phonon lines sharpen as temperature decreases. With the width axis relabelled as temperature, the constant area curves show temperature dependence very similar to that of the sharp line of Figure 6.5.

The Lorentzian line, having wider wings, should show less loss of intensity when narrow and strong than the Gaussian. It can be seen that the true intensity curves fall closer to the Intensity axis for the Lorentzian case, verifying that of two lines showing the same intensity reduction, the

Lorentzian is narrower. The apparently high integrated intensity curves for the Gaussian are deceptive, since the wings of a Lorentzian contribute to its area, with apparent reduction in intensity for the constant area curve.

```
 A1(D2) A40 TRIG        3    1
   1000000    1000000    1040400
 10000000.E-01 00000000.E-99
 10202000.E-01 00000000.E-99 13659754.E-08
 10404000.E-01 29814237.E-08-25453450.E-08 10244815.E-08
   1040403    1040403    1040403
 10404030.E-01-11952285.E-08
   3010000    3010000    3030403
 30100000.E-01 00000000.E-99
 30102000.E-01 00000000.E-99 00000000.E-99
 30302000.E-01 00000000.E-99-12777530.E-08-12521442.E-08
 30303030.E-01 00000000.E-99 00000000.E-99 00000000.E-99-19920475.E-09
 30304000.E-01-12171612.E-08 61475922.E-09 98580787.E-09 00000000.E-99
-15367224.E-08
 30304030.E-01 00000000.E-99 00000000.E-99 00000000.E-99 17251636.E-08
 00000000.E-99 17928428.E-08
 A1(D2) A43 TRIG        2    1
   1000000    1000000    1040403
 10000000.E-01 00000000.E-99
 10202000.E-01 00000000.E-99 00000000.E-99
 10404000.E-01 00000000.E-99 00000000.E-99 00000000.E-99
 10404030.E-01 42163700.E-08 12598815.E-08-16903084.E-08 00000000.E-99
   3010000    3010000    3030403
 30100000.E-01 00000000.E-99
 30102000.E-01 00000000.E-99 00000000.E-99
 30302000.E-01 00000000.E-99 00000000.E-99 00000000.E-99
 30303030.E-01 00000000.E-99-15811388.E-08 30988988.E-08 00000000.E-99
 30304000.E-01 00000000.E-99 00000000.E-99 00000000.E-99-24397499.E-08
 00000000.E-99
 30304030.E-01-17213258.E-08-30429030.E-09-48794999.E-09 00000000.E-99
 25354626.E-08 00000000.E-99
 A1(D2) A20 TRIG        3    1
   1000000    1000000    1040400
 10000000.E-01 00000000.E-99
 10202000.E-01 40000000.E-08 10244815.E-08
 10404000.E-01 00000000.E-99 18326484.E-08-34149388.E-08
   1040403    1040403    1040403
 10404030.E-01 11952285.E-08
   3010000    3010000    3030403
 30100000.E-01 00000000.E-99
 30102000.E-01-23664318.E-08 16733200.E-08
 30302000.E-01 25298220.E-08-51110121.E-09-81958532.E-09
 30303030.E-01 00000000.E-99 00000000.E-99 00000000.E-99 89642139.E-09
 30304000.E-01 00000000.E-99 26557599.E-08 11829694.E-09 00000000.E-99
-85373466.E-09
 30304030.E-01 00000000.E-99 00000000.E-99 00000000.E-99-51754913.E-09
 00000000.E-99 29880714.E-09
```

```
E(D2)  A40 TRIG        4    1
  1020201   1020201   1040402
10202010.E-01-91065029.E-09
10202020.E-01 00000000.E-99 22766258.E-09
10404010.E-01-69707141.E-09 00000000.E-99 51224082.E-09
10404020.E-01 00000000.E-99 29574236.E-08 00000000.E-99-62607211.E-09
  1040404   1040404   1040404
10404040.E-01 79681906.E-09
  3010101   3010101   3030402
30101010.E-01 00000000.E-99
30102010.E-01 00000000.E-99 00000000.E-99
30102020.E-01 00000000.E-99 00000000.E-99 00000000.E-99
30302010.E-01 00000000.E-99 85183538.E-09 00000000.E-99 83476282.E-09
30302020.E-01 00000000.E-99 00000000.E-99-21295884.E-09 00000000.E-99
-20869070.E-09
30303010.E-01 59761429.E-09 99602375.E-09 00000000.E-99-19521227.E-08
00000000.E-99-66401588.E-10
30303020.E-01 00000000.E-99 00000000.E-99-62994076.E-09 00000000.E-99
12346308.E-08 00000000.E-99 46481111.E-09
30304010.E-01 11785112.E-08 16835873.E-09 00000000.E-99 26997460.E-09
00000000.E-99-15152286.E-08 00000000.E-99-76836123.E-09
30304020.E-01 00000000.E-99 00000000.E-99-71428571.E-09 00000000.E-99
-11454052.E-08 00000000.E-99-11293848.E-08 00000000.E-99 93910811.E-09
  3030404   3030404   3030404
30304040.E-01-11952285.E-08
E(D2)  A43 TRIG        2    1
  1020201   1020201   1040404
10202010.E-01 00000000.E-99
10202020.E-01 13468699.E-08 00000000.E-99
10404010.E-01 00000000.E-99 24743582.E-08 00000000.E-99
10404020.E-01-29160589.E-08 00000000.E-99 47619047.E-09 00000000.E-99
10404040.E-01-30860669.E-08 00000000.E-99-12598815.E-08 00000000.E-99
00000000.E-99
  3010101   3010101   3030404
30101010.E-01 00000000.E-99
30102010.E-01 00000000.E-99 00000000.E-99
30102020.E-01 00000000.E-99 00000000.E-99 00000000.E-99
30302010.E-01 00000000.E-99 00000000.E-99-12598815.E-08 00000000.E-99
30302020.E-01 00000000.E-99-12598815.E-08 00000000.E-99-12346308.E-08
00000000.E-99
30303010.E-01 00000000.E-99 00000000.E-99 11785112.E-08 00000000.E-99
23097828.E-08 00000000.E-99
30303020.E-01 11180339.E-08-37267796.E-09 00000000.E-99 73041747.E-09
00000000.E-99 24845198.E-09 00000000.E-99
30304010.E-01 00000000.E-99 00000000.E-99-59761429.E-09 00000000.E-99
95831479.E-09 00000000.E-99 18898223.E-08 00000000.E-99
30304020.E-01-98601324.E-09 70429514.E-09 00000000.E-99 11293848.E-08
00000000.E-99-84515422.E-09 00000000.E-99-71428571.E-09 00000000.E-99
30304040.E-01 74535595.E-09 74535595.E-09 00000000.E-99 11952285.E-08
00000000.E-99 22360679.E-08 00000000.E-99 18898223.E-08 00000000.E-99
00000000.E-99
```

```
 E(D2) A20 TRIG        4    1
  1020201   1020201   1040402
10202010.E-01 51224082.E-09
10202020.E-01 00000000.E-99-10244815.E-08
10404010.E-01 16729713.E-08 0000000.E-99-29026979.E-08
10404020.E-01 00000000.E-99 11829694.E-08 00000000.E-99-13659754.E-08
  1040404   1040404   1040404
10404040.E-01 47809143.E-08
  3010101   3010101   3030402
30101010.E-01 83666002.E-09
30102010.E-01 25099800.E-08 83666002.E-09
30102020.E-01 00000000.E-99 00000000.E-99-16733200.E-08
30302010.E-01 17888543.E-08-25555060.E-09 00000000.E-99-40979265.E-09
30302020.E-01 00000000.E-99 00000000.E-99 51110121.E-09 00000000.E-99
81958532.E-09
30303010.E-01 19123656.E-08 95618284.E-09 00000000.E-99-38332592.E-09
00000000.E-99-53785286.E-09
30303020.E-01 00000000.E-99 00000000.E-99 15118578.E-08 00000000.E-99
-60609148.E-09 00000000.E-99 00000000.E-99
30304010.E-01 00000000.E-99 24243659.E-08 00000000.E-99 10798984.E-09
00000000.E-99-25253811.E-09 00000000.E-99-72567449.E-09
30304020.E-01 00000000.E-99 00000000.E-99 17142857.E-08 00000000.E-99
76360352.E-10 00000000.E-99-45175393.E-09 00000000.E-99-34149388.E-09
  3030404   3030404   3030404
30304040.E-01 11952285.E-08



A2(D2) A40 TRIG        3    1
  1040403   1040403   1040403
10404030.E-01-11952285.E-08
  3010100   3010100   3030300
30101000.E-01 00000000.E-99
30303000.E-01-97589999.E-09-39840952.E-09
  3030303   3030303   3030403
30303030.E-01-19920475.E-09
30304030.E-01 17251636.E-08 17928428.E-08
A2(D2) A43 TRIG        2    1
  1040403   1040403   1040403
10404030.E-01
  3010100   3010100   3030403
30101000.E-01 0000000.E-99
30303000.E-01 00000000.E-99 00000000.E-99
30303030.E-01-91287088.E-09 74535595.E-09 00000000.E-99
30304030.E-01-15811388.E-08 12909944.E-08 00000000.E-99 00000000.E-99
A2(D2) A20 TRIG        3    1
  1040403   1040403   1040403
10404030.E-01 11952285.E-08
  3010100   3010100   3030300
30101000.E-01-16733200.E-08
30303000.E-01 23421599.E-08-71713715.E-09
  3030303   3030303   3030403
30303030.E-01 89642139.E-09
30304030.E-01-51754913.E-09 29880714.E-09
```

```
S-0 (D2)                          100
   3 1 0      3 1 0      1 4 4
       3 1 0  -1.
       3 1 1                -0.5
       3 1 2                              0.5
       3 3 2                                            -2.
       3 3 3
       -0.5
       3 3 4
              1.5
       1 0 0  -2.449489742

       1 2 2                              1.449137674   -1.549193338

       1 4 4
              1.0
B(D2)                           10000
   3 3        3 3        1 0
       3 3    -8.
       3 1                  7.
       1 4                                4.
       1 2                                              -3.
       1 0
 14.
C(D2)                           10000
   1 4        1 4        1 0
       1 4    2.
       1 2                  2.
       1 0                                7.
```

PARAMETER TRANSFORMATIONS

$$\begin{bmatrix} \Delta \\ v \\ v' \end{bmatrix} = \begin{bmatrix} -0.15493704 & 0.37037037 & 0.0 \\ 0.26560636 & 0.22222222 & -0.35856868 \\ 0.09390603 & 0.07856742 & 0.16903085 \end{bmatrix} \begin{bmatrix} A^4_0 \\ A^4_3 \\ A^2_0 \end{bmatrix}$$

$$\begin{bmatrix} A^4_0 \\ A^4_3 \\ A^2_0 \end{bmatrix} = \begin{bmatrix} -1.6733200 & 1.5936381 & 3.3806170 \\ 2.0 & 0.66666666 & 1.41421356 \\ 0.0 & -1.1952286 & 3.3806170 \end{bmatrix} \begin{bmatrix} \Delta \\ v \\ v' \end{bmatrix}$$

APPENDIX FIVE

CELL THEORY PROGRAM

In a dense monatomic liquid neighbour atoms tend to pack together closely, which can result in short range order. A model utilising this is the cell model of the liquid state, which consideres each atom as surrounded by twelve others in face-centred cubic coordination[63]. No order of longer range than this is assumed. The forces acting between the atoms restrain the central atom into a definite volume, in which it is free to move in a potential well $\psi(\underline{r})$ due to the interatomic interactions. If the well is localised near the origin, the atom will have restricted movement, but if the well is wide, the atom can move throughout the whole of the volume inside the planes bisecting the distances between the origin and the nearest neighbour positions.

This freedom of movement can be expressed in terms of a quantity called the Free Volume v_f, defined as

$$v_f = \int e^{-\frac{\psi(\underline{r})}{kT}} d\tau$$

where the integral is taken over the whole dodecahedral cell, and the origin is taken as the zero of energy. If ψ remains small over the cell, the integral will approach the cell volume, if ψ increases sharply away from the origin v_f

will be decreased.

The theory is normally applied to liquids such as Argon, where the interatomic potential has the form

$$\phi(r) = \varepsilon \left[\left(\frac{a}{r}\right)^{12} - 2\left(\frac{a}{r}\right)^{6} \right]$$

and the energy term $\psi(x,y,z) = \sum_i \left[\phi_i(x,y,z) - \phi_i(0,0,0)\right]$, with i ranging over the neighbours. The two parameters can be absorbed by defining reduced temperature as kT/ε, and taking a as the unit of length. The variables in the model are then the reduced temperature and the cell volume.

The integration is performed from the centre outwards over a regular grid for $x,y,z > 0$, stopping when significance is lost or the limit of integration is reached. The derivative $w\frac{\partial v}{\partial w}f$ is calculated at the same time. The two cases of twelve and eleven neighbours are considered together, for five temperatures, This sharing of arithmetic between 20 calculations results in considerable time saving.

Several sense switch options are available. If Sw 1 is turned on before calculation begins, x,y and z values are accepted and integrand values calculated for that point. This facility is useful for deciding what grid step to use. If Sw 1 is turned on during calculation, the values of the running sums are typed out. Sw 2 is used during integration to allow for the possibility that a significant contribution to the integral may come from the region near x=y, which passes between atoms. If the switch is on, this region is tested for each integration along an x line. Sw 3 is used for input/output of a partial calculation. If the switch is turned on, intermediate output is punched, and can be reread later if Sw 3 is on at input time.

PROGRAM LISTINGS

Cell Theory Integration

```
*0810
C     FORTRAN 2 VERSION OF CELL THEORY
C     SPS APPENDIX TO ATTEMPT SPEEDING UP
C     FIVE TEMPERATURES IN ASCENDING ORDER
C
C     SW1
C            IF TURNED ON DURING CALCULATION GIVES PRESENT
C            VALUES OF SUMS AND CONTINUES
C     SW2    ON MID POINT SIGNIFICANCE CHECK
C     SW3    OFF SEGMENT INPUT,  ON NORMAL INPUT
C            GIVES SEGOUT IF TURNED ON DURING CALCULATION
C     SW4    OFF NORMAL INPUT TYPE,  ON CARDS
C
C
      COMMON IXP1,IYM1,IXP2,IXM2,IX2,
     1 IYP1,IYM1,IYP2,IYM2,IY2,IZPR,IZMR,IZ2,
     2 S6T1,S6T2,S6T3,S6T4,S6T5,
     3 S12T1,S12T2,S12T3,S12T4,S12T5
      COMMON T1SA,T2SA,T3SA,T4SA,T5SA,
     1 T1TWA,T2TWA,T3TWA,T4TWA,T5TWA,
     2 T1SB,T2SB,T3SB,T4SB,T5SB,
     3 T1TWB,T2TWB,T3TWB,T4TWB,T5TWB
      COMMON T1SF,T2SF,T3SF,T4SF,T5SF,
     1 T1TWF,T2TWF,T3TWF,T4TWF,T5TWF
C     WORKING VARIABLES
      COMMON WEXP,WD,F10,LQ,LR
C     FINAL VALUES
      COMMON S1F,S2F,S3F,S4F,S5F,
     1 S1A,S2A,S3A,S4A,S5A,
     2 S1B,S2B,S3B,S4B,S5B
      COMMON SD1F,SD2F,SD3F,SD4F,SD5F,
     1 SD1A,SD2A,SD3A,SD4A,SD5A,
     2 SD1B,SD2B,SD3B,SD4B,SD5B
C     TEMPERATURES
      COMMON T1,T2,T3,T4,T5
C     MORE WORKING VARIABLES
      COMMON W,MP,MQ,MR,L,LP,
     1MTR,MPS,IG,MBP,MBQ,MBR
      EQUIVALENCE (IXP1,I)
C
    1 IF(SENSE SWITCH 3)2,902
  902 CALL SEGIN
      GO TO 46
    2 CALL INPUT
 20   IF(SENSE SWITCH 1)801,6
    6 ACCEPT 506,IG
C     FIND SQUARES OF DISTANCES
      MBP=IG/2
      MBQ=MBP
      MBR=MBP
      MR=MBR
   43 WW=MR
      MTR=WW*1.4142136-2.E+09
      LR=1
      IZ2=MR
      CALL MULT(IZ2)
      IZPR=MR+1414213562
      CALL MULT(IZPR)
      IZMR=MR-1414213562
      CALL MULT(IZMR)
      MQ=MBQ
   42 L=1
      MPS=0
      LQ=1
      IYP2=20000 00000+MQ
      CALL MULT(IYP2)
      IYP1=10000 00000+MQ
      CALL MULT(IYP1)
      IY2=MQ
      CALL MULT(IY2)
      IYM1=10000 00000-MQ
      CALL MULT(IYM1)
      IYM2=20000 00000-MQ
      CALL MULT(IYM2)
      MP=MBP
   41 LP=1
      IF(SENSE SWITCH 3)989,46
   46 IXP2=20000 00000+MP
      CALL MULT(IXP2)
      IXP1=10000 00000+MP
      CALL MULT(IXP1)
      IX2=MP
      CALL MULT(IX2)
      IXM1=MP-10000 00000
      CALL MULT(IXM1)
      IXM2=MP-20000 00000
      CALL MULT(IXM2)
C
      CALL COORD
C
C     WE NOW HAVE 30 FG NUMBERS
   26 CALL USE(T1TWF,T1SF,S1F,SD1F
      CALL USE(T2TWF,T2SF,S2F,SD2F
      CALL USE(T3TWF,T3SF,S3F,SD3F
      CALL USE(T4TWF,T4SF,S4F,SD4F
      CALL USE(T5TWF,T5SF,S5F,SD5F
      CALL USE(T1TWA,T1SA,S1A,SD1A
      CALL USE(T2TWA,T2SA,S2A,SD2A
      CALL USE(T3TWA,T3SA,S3A,SD3A
      CALL USE(T4TWA,T4SA,S4A,SD4A
      CALL USE(T5TWA,T5SA,S5A,SD5A
      CALL USE(T1TWB,T1SB,S1B,SD1B
      CALL USE(T2TWB,T2SB,S2B,SD2B
      CALL USE(T3TWB,T3SB,S3B,SD3B
      CALL USE(T4TWB,T4SB,S4B,SD4B
      CALL USE(T5TWB,T5SB,S5B,SD5B
C     NEXT POINT
      IF(SENSE SWITCH 1)899,12
   12 IF(MP+IG+MQ+MTR)8,9,9
    8 IF(MP-1000000000)13,9,9
C     LAST POINT ANY USE
   13 GO TO (102,14),LP
   14 GO TO (15,15,108),L
C
C     OUTSIDE LIMIT
    9 GO TO (17,110,13 ),L
C
C     MID-PLANE ROUTINE
  102 IF(SENSE SWITCH 2)109,17
  109 GO TO (103,110,17),L
  103 IF(MP-MQ)104,17,17
  104 MPS=MP
      IF(MQ+MQ+MTR)106,107,107
  106 MP=MQ
      L=2
      GO TO 41
  107 MP=-MTR-MQ
      L=3
      GO TO 41
C     BACKSPACE ROUTINE
  110 L=3
      MP=MQ-IG
      GO TO 41
C     CONTINUING
  108 MP=MP-IG
      IF(MP-MPS)17,17,41
C
C     INCREMENT MP
   15 MP=MP+IG
      GO TO 41
C     TEST AND INCREMENT MQ
   17 GO TO (39,31),LQ
   31 IF(MQ-1000000000)32,39,39
   32 MQ=MQ+IG
      GO TO 42
C     TEST AND INCREMENT MR
   39 GO TO (701,38),LR
   38 IF(MR-1414213562)37,701,701
   37 MR=MR+IG
      GO TO 43
  701 CALL FNOUT
      GO TO 1
  801 CALL SEEK
      GO TO 43
  989 CALL SEGOUT
      STOP
  899 CALL FIND
C     INTEGRATING OR LOOKING
      GO TO (12,898),I
  898 IF(SENSE SWITCH 2)2,20
  506 FORMAT(I10)
      END
```

```
*0810
      SUBROUTINE INPUT
      DIMENSION ID1(13),D2(32),T(5),S(10),ANS(30),M(3)
      COMMON ID1,S,D2,WW,I,LR,ANS,T,W,M,L,LC,MTR,MPS,IG
    4 PRINT 503
      ACCEPT 504,W,(T(I),I=1,5)
    5 WW=W*W/32.
      DO 1 I=6,10
    1 S(I)=1./(WW*T(I-5))
      WW=WW*WW
      DO 2 I=1,5
    2 S(I)=1./(WW*T(I))
      PRINT 507
      PAUSE
C     NOW INITIALISE
   85 DO 10I=1,30
   10 ANS(I)=0.
      IG=0.
      RETURN
  501 FORMAT(6F10.3)
  503 FORMAT(7HW,TEMPS)
  504 FORMAT(F10.3)
  507 FORMAT(7HSW3 OFF)
      END

*0810
      SUBROUTINE SEEK
      DIMENSION ID1(96), ID2(5)
      COMMON ID1, MR, ID2,MBP,MBQ
      PRINT 508


  806 ACCEPT 506,MBP,MBQ,MR
  808 RETURN
  506 FORMAT(I10)
  508 FORMAT(//5HY/Y/Z)
  513 FORMAT(3I10)
      END

*0810
      SUBROUTINE FIND
C     TO TYPE OUT RUNNING SUMS IF SW 1 ON
      DIMENSION ID1(55),S(5,6),T(5),ID2(4)
      COMMON IRET,I,J,ID1,S,T,W,
     1MP,MQ,MR,ID2,IG
      PRINT 10,MP,MQ,MR,W
   10 FORMAT(/4H  X=I10,4H  Y=I10,4H  Z=I10/2HW=E14.7/
     14H   T 8X 3HV10 1 X 3HV A 12X 2HVC)
      DO 2 I=1,5
      IF(SENSE SWITCH 1)2,3
    2 PRINT 20,T(I),(S(I,J),J=1,6)
    3 IF(IG)5,4,5
    5 IRET=1
      RETURN
    4 IRET=2
      PAUSE
      DO 6 I=1,5
      DO 6 J=1,6
    6 S(I,J)=0.
      RETURN
   20 FORMAT(F6.3,3E15.7/6X,3E15.7)
      END

*0810
      SUBROUTINE USE (A,B,P,Q)
      DIMENSION D(52), OD(40)
      COMMON IV,D,WEXP,WD,FID,LQ,LR,DD,LP
C     ARGUMENTS IN COMMON SO NO FLAGS NEEDED
C     ON PATCH INSTRUCTIONS
      WEXP=2.*B-A
      WD=A-B
      IV=WEXP
C     INTEGER VALUE OF EXPONENT
      IV=-15-IV
C     IF POSITIVE,EXP(-WEXP) INSIGNIFICANT
      IF(IV)1,1,2
C     NOW TEST WD TERM
C     HM WD,23,10,EXPONENT ONLY
    2 PAUSE 11111
C     S IV,00098,,NOW READY TO TEST WD
      PAUSE 11111
      IF(IV)1,1,3
C     ONE OR BOTH USEFUL
    1 LP=2
      LQ=2
      LR=2
      FID=EXPF(WEXP)
      P=P+FID
      Q=Q+WD*FID
      RETURN
    3 LP=1
      RETURN
      END

*0810
      SUBROUTINE FNOUT
      DIMENSION D1(38),F(5),A(5),B(5),FD(5),FA(5),FB(5),T(5),ID2(6)
      DIMENSION VE(5),VF(5),DVE(5),DVF(5)
      COMMON VF,VE,DVF,DVE,D1,F,A,B,FD,FA,FB,T,W,I,ID2,IG
      EQUIVALENCE (GRIV,D1(35)),(GRIS,D1(37))
      GRIV=IG/100
      GRIS=GRIV/10000000.
      GRIV=GRIS*GRIS*GRIS*W*.176776695
      IF(SENSE SWITCH 1) 703,702
  702 PRINT 517,GRIS
      PRINT 518,W
  703 PUNCH 517,GRIS
      PUNCH 518,W
      DO 3 I=1,5
      VF(I)=8.*GRIV*F(I)
      VE(I) =4.*GRIV*(A(I)+B(I))
      DVF(I)=VF(I)+32.*GRIV*FD(I)
    1 DVE(I)=VE(I)+16.*GRIV*(FA(I)+FB(I))
      IF(SENSE SWITCH 1)4,2
    2 PRINT 519,T(I),VF(I),VE(I)
      PRINT 520,DVF(I),DVE(I)
    4 PUNCH 519,T(I),VF(I),VE(I),W,IG
    3 PUNCH 521,T(I),DVF(I),DVE(I),W,IG
      PAUSE
      RETURN
  517 FORMAT(11HGRID INCRT=F10.6)
  518 FORMAT(2HW=F10.6,7X,8HV12/DV12 10X,8HV11/DV11 )
  519 FORMAT(2HT=F10.6,4X,E14.7,3X,E14.7,8X,E14.8,I11)
  520 FORMAT(16X,E14.7,3X,E14.7//)
  521 FORMAT(2X,F10.6,4X,E14.7,3X,E14.7,8X,E14.8,I11)
      END

*0810
      SUBROUTINE SEGOUT
      DIMENSION ID1(5),D1(30)
      COMMON ID1,
     1IYP1,IYM1,IYP2,IYM2,IY2,IZPR,IZMR,IZ2,
     2S6T1,S6T2,S6T3,S6T4,S6T5,
     3S12T1,S12T2,S12T3,S12T4,S12T5
      COMMON D1
      COMMON NSEK,ISWCH,D2,LQ,LR
C     FINAL VALUES
      COMMON S1F,S2F,S3F,S4F,S5F,
     1 S1A,S2A,S3A,S4A,S5A,
     2 S1B,S2B,S3B,S4B,S5B
      COMMON SD1F,SD2F,SD3F,SD4F,SD5F,
     1 SD1A,SD2A,SD3A,SD4A,SD5A,
     2 SD1B,SD2B,SD3B,SD4B,SD5B
C     TEMPERATURES
      COMMON T1,T2,T3,T4,T5
C     MORE WORKING VARIABLES
      COMMON W,MP,MQ,MR,L,LP,
     1MTR,MPS,IG,MBP,MBQ,MBR
      NSEK=1
      PUNCH 510, MP,MQ,MR,MTR,MPS,IG,NSEK
      NSEK=2
      PUNCH 510, IZ2,IZPR,IZMR,IYP2,IYP1,IY2,NSEK
      NSEK=3
      PUNCH 510,IYM1,IYM2,L,LP,LQ,LR,NSEK
      NSEK=4
      PUNCH 509,S1F,S2F,S3F,S4F,S5F,NSEK
      NSEK=5
      PUNCH 509,S1A,S2A,S3A,S4A,S5A,NSEK
      NSEK=6
      PUNCH 509,S1B,S2B,S3B,S4B,S5B,NSEK
      NSEK=7
      PUNCH 509,SD1F,SD2F,SD3F,SD4F,SD5F,NSEK
      NSEK=8
      PUNCH 509,SD1A,SD2A,SD3A,SD4A,SD5A,NSEK
      NSEK=9
      PUNCH 509,SD1B,SD2B,SD3B,SD4B,SD5B,NSEK
      NSEK=10
      PUNCH 509,S6T1,S6T2,S6T3,S6T4,S6T5,NSEK
      NSEK=11
      PUNCH 509,S12T1,S12T2,S12T3,S12T4,S12T5,NSEK
      NSEK=12
      PUNCH 509,T1,T2,T3,T4,T5,NSEK
      IF(SENSE SWITCH 2)1,2
    1 ISWCH=1
      GO TO 3
    2 ISWCH=2
    3 NSEK=13
      PUNCH 512,W,ISWCH,NSEK
      STOP
  509 FORMAT(5E14.8,I10)
  510 FORMAT(6I11,3X,I11)
  512 FORMAT(E14.8,6X,I10,39X,I11)
      END
```

```
*0810
      SUBROUTINE SEGIN
      DIMENSION ID1(5),D1(30)
      COMMON ID1,
     1IYP1,IYM1,IYP2,IYM2,IY2,IZPR,IZMR,IZ2,
     2S6T1,S6T2,S6T3,S6T4,S6T5,
     3S12T1,S12T2,S12T3,S12T4,S12T5
      COMMON D1
      COMMON NSEK,ISWCH,D2,LQ,LR
C     FINAL VALUES
      COMMON S1F,S2F,S3F,S4F,S5F,
     1 S1A,S2A,S3A,S4A,S5A,
     2 S1B,S2B,S3B,S4B,S5B
      COMMON SD1F,SD2F,SD3F,SD4F,SD5F,
     1 SD1A,SD2A,SD3A,SD4A,SD5A,
     2 SD1B,SD2B,SD3B,SD4B,SD5B
C     TEMPERATURES
      COMMON T1,T2,T3,T4,T5
C     MORE WORKING VARIABLES
      COMMON W,MP,MQ,MR,L,LP,
     1MTR,MPS,IG,MBP,MBQ,MBR
   97 READ 510,MP,MQ,MR,MTR,MPS,IG,NSEK
      MBP=IG/2
      MBQ=MBP
      MBR=MBP
      IF(NSEK-1)99,1,99
    1 READ 510, IZ2,IZPR,IZMR,IYP2,IYP1,IY2,NSEK
      IF(NSEK-2)99,2,99
    2 READ 510,IYM1,IYM2,L,LP,LQ,LR,NSEK
      IF(NSEK-3)99,3,99
    3 READ 509,S1F,S2F,S3F,S4F,S5F,NSEK
      IF(NSEK-4)99,4,99
    4 READ 509,S1A,S2A,S3A,S4A,S5A,NSEK
      IF(NSEK-5)99,5,99
    5 READ 509,S1B,S2B,S3B,S4B,S5B,NSEK
      IF(NSEK-6) 99,6,99
    6 READ 509,SD1F,SD2F,SD3F,SD4F,SD5F,NSEK
      IF(NSEK-7)99,7,99
    7 READ 509,SD1A,SD2A,SD3A,SD4A,SD5A,NSEK
      IF(NSEK-8)99,8,99
    8 READ 509,SD1B,SD2B,SD3B,SD4B,SD5B,NSEK
      IF(NSEK-9)99,9,99
    9 READ 509,S6T1,S6T2,S6T3,S6T4,S6T5,NSEK
      IF(NSEK-10)99,10,99
   10 READ 509,S12T1,S12T2,S12T3,S12T4,S12T5,NSEK
      IF(NSEK-11)99,11,99
   11 READ 509,T1,T2,T3,T4,T5,NSEK
      IF(NSEK-12) 99,12,99
   12 READ 512,W,ISWCH,NSEK
      IF(NSEK-13)99,13,99
   99 PRINT 514
      PAUSE
      GO TO 97
   13 GO TO (14,15),ISWCH
   14 PRINT 516
   98 PAUSE
      RETURN
   15 PRINT 515
      GO TO 98
  509 FORMAT(5E14.8,I10)
  510 FORMAT(6I11,3X,I11)
  512 FORMAT(F14.8,6X,I10,39X,I11)
  514 FORMAT(20HCARD OUT OF SEQUENCE)
  515 FORMAT(17HPROG SWITCHES OFF)
  516 FORMAT(16HSW2 ON, REST OFF)
      END
```

```
*0810
      SUBROUTINE MULT(NUM)
C     FOR SQUARING TEN-FIGURE NUMBERS
      PAUSE
      PAUSE
      PAUSE
C     M NUM,NUM,0126711
C     SF 00081,,,SIZE OF NUMBER LIMITED
C     TF NUM,00090,026
      RETURN
      END
```

Object deck altered

```
*0810
      SUBROUTINE COORD
      PAUSE
      RETURN
      END
```

Header cards added to following SPS program

```
01010 *         APPENDIX WRITTEN AS SIMULATED
01020 *         FORTRAN SUBROUTINE 18/7/64
01030 *
01040 *         DISTANCE FINDING
01050       DORG 12050
01060 INIT  AM   INIT-1,1,0210
01065       TF   RS6,ZERO-3,0127
01070       TF   RS12,ZERO ,0127
01080 FIRST TF   L6,ZERO-4 ,0127
01090       A    L6  , XP1 ,02
01100       A    L6  , YP1 ,02
01110       A    L6  , ZPR ,02
01120       BTM  RECIP,*+12,0127
01130 TWO   TF   L6,ZERO-4 ,0127
01140       A    L6  , XP1 ,02
01150       A    L6  , YP1 ,02
01160       A    L6  , ZMR ,02
01170       BTM  RECIP,*+12,0127
01180 THREE TF   L6,ZERO-4 ,0127
01190       A    L6  , XP1 ,02
01200       A    L6  , YM1 ,02
01210       A    L6  , ZPR ,02
01220       BTM  RECIP,*+12,0127
01230 FOUR  TF   L6,ZERO-4 ,0127
01240       A    L6  , XP1 ,02
01250       A    L6  , YM1 ,02
02010       A    L6  , ZMR ,02
02020       BTM  RECIP,*+12,0127
02030 FIVE  TF   L6,ZERO-4 ,0127
02040       A    L6  , XM1 ,02
02050       A    L6  , YP1 ,02
02060       A    L6  , ZPR ,02
02070       BTM  RECIP,*+12,0127
02080 SIX   TF   L6,ZERO-4 ,0127
02090       A    L6  , XM1 ,02
02100       A    L6  , YP1 ,02
02110       A    L6  , ZMR ,02
02120       BTM  RECIP,*+12,0127
02130 SEVEN TF   L6,ZERO-4 ,0127
02140       A    L6,   XM1 ,02
02150       A    L6,   YM1 ,02
02160       A    L6,   ZPR ,02
02170       BTM  RECIP,*+12,0127
02180 EIGHT TF   L6,ZERO-4 ,0127
02190       A    L6  , XM1 ,02
02200       A    L6  , YM1 ,02
02210       A    L6  , ZMR ,02
02220       BTM  RECIP,*+12,0127
02230 NINE  TF   L6,ZERO-4 ,0127
02240       A    L6  ,  Y2 ,02
02250       A    L6  , YP2 ,02
03010       A    L6  ,  Z2 ,02
03020       BTM  RECIP,*+12,0127
03030 TEN   TF   L6,ZERO-4 ,0127
03040       A    L6  ,  Y2 ,02
03050       A    L6  , YM2 ,02
03060       A    L6  ,  Z2 ,02
03070       BTM  RECIP,*+12,0127
03080 *     ZEROAT ORIGIN FOR ELEVEN
03090       S    RS6  , D6 ,0127
03100       S    RS12 ,D12 ,0127
03110 *         SAVE SUMS
03120       TF   R10 , RS6 ,0127
03130       TF   T10 ,RS12 ,0127
03140 ELEVA TF   L6,ZERO-4 ,0127
03150       A    L6  , XP2 ,02
03160       A    L6  ,  Y2 ,02
03170       A    L6  ,  Z2 ,02
03180       BTM  RECIP,*+12,0127
03190 *         NOW FLOAT
03200       TFM  FLOAT+23,39767,027
03210       BTM  FLOAT,*+12,0127
03220 ELEVB TF   L6,ZERO-4 ,0127
03230       TF   RS6 , R10 ,0127
03240       TF   RS12, T10 ,0127
03250       A    L6  , XM2 ,02
04010       A    L6  ,  Y2 ,02
04020       A    L6  ,  Z2 ,02
04030       BTM  RECIP,*+12,0127
04040 *         SAVE SUMS AGAIN
04050       TF   R10 , RS6 ,0127
04060       TF   T10 , RS12,0127
04070 *         FLOAT NEW SUMS
04080       TFM  FLOAT+23,39667,027
04090       BTM  FLOAT,*+12,0127
04100       TF   RS6 , R10 ,0127
04110       TF   RS12, T10 ,0127
04120 *     ZEROAT ORIGIN FOR TWELVE
04130       S    RS6 ,  C6 ,0127
04140       S    RS12, C12 ,0127
04150 TWELVE TF  L6,ZERO-4 ,0127
04160       A    L6  , XP2 ,02
04170       A    L6  ,  Y2 ,02
04180       A    L6  ,  Z2 ,02
04190       BTM  RECIP,*+12,0127
04200 *         FLOAT LAST SET
04210       TFM  FLOAT+23,39567,027
04220       BTM  FLOAT,*+12,0127
04230 *         NOW FINISHED, RETURN
04240 RETURN B   INIT-1,,026
04250 *
```

```
05010 *
05020 *          STORAGE ALLOCATION
05030 *
05040 XP1     DS    ,39999
05050 XM1     DS    ,39989
05060 XP2     DS    ,39979
05070 XM2     DS    ,39969
05080 X2      DS    ,39959
05090 YP1     DS    ,39949
05100 YM1     DS    ,39939
05110 YP2     DS    ,39929
05120 YM2     DS    ,39919
05130 Y2      DS    ,39909
05140 ZPR     DS    ,39899
05150 ZMR     DS    ,39889
05160 Z2      DS    ,39879
05170 ZERO    DC    15,0
05180         DC     1,@
05190 RS6     DS    12
05200         DC     1,@
05210 RS12    DS    15
05220         DC     1,@
05230 L6      DS    11
05240         DC     1,@
05250 R10     DS    12
06010 T10     DS    15
06020 ST06    DS    12
06030 ST012   DS    15
06040 ONE     DC    10 , 1000000000
06050 C6      DC     9 , 156250000
06060 06      DC    10 , 1718750000
06070 C12     DC    10 , 2441406250
06080 012     DC    11 , 26855468750
06090 WORK    DS    11
06100 SPACE   DS     5
06110 *          ROOM FOR Q OF BTM
06120 *
06130 *
07010 *          SUBROUTINES
07020 *
07030 RECIP   BD    R1 , L6-10,0127
07040         BD    R2 , L6-9 ,0127
07050         TR    L6-10,L6-9,0127
07060 *          POSITION NUMBERS FOR DIVISION
07070         TDM   L6    , 0 ,02
07080         B     R2,,02
07090 R1      TF    L6 , L6-1 ,0127
07100 R2      SF    L6-9     , ,02
07110 *          NOW TEN SIG FIGS
07120         TF    00079,ZERO,17,CLEAR DIV AREA
07130         LD    00089, ONE,17
07140         D     00088, L6 ,17
07150         BD    FLUKE,0079,02
07160         SF    00080
07170         TF    L6, 00089 ,02,TEN SIG FIG
07180         M     L6    , L6 ,0127
07190         TF    WORK,00089,02
07200         M     L6 , WORK ,0127
07210         BD    R3 , L6-10,0127
07220         BNF   R4 , L6-10,0127
07230         TF    ST06,00089,02
07240 RR      M     ST06, ST06,0127
07250         A     RS12,00092,02
08010 RRR     A     RS6, ST06 ,0127
08020         B     RECIP-1 , ,026
08030 R3      TF    ST06,00086,02
08040         B     RR       , ,02
08050 R4      SF    00082
08060         BO    142,81
08070         TF    ST06,00092,02
08075         TF    00079,ZERO-8,127
08080         B     RR       , ,02
08090 FLUKE   BNF   STOP,L6-10,0127
08100         BD    FT , L6-10,0127
08110         TF    ST06-1,ONE,0127
08120         TDM   ST06  , 0 ,02
08130         TF    ST012,ONE-5,0127
08140         TF    ST012-4,ONE,0127
08150         A     RS12,ST012,0127
08160         B     RRR      , ,02
08170 STOP    H
08180         B     *-12     , ,02
08181 FT      TF    ST06,ONE-2,0127
08182         A     RS12,ONE-2,0127
08183         B     RRR ,,02
08190 *
08200 *
08210 FLOAT   TFM   X      , 2 ,0210
08220 X       DS    ,*-2
08230         TFM   BACK      , ,02
08240         TFM   EXT,RS6-11,0127
08250         MF    SAFLAG,RS6,0127
09010         BTM   F1 , 39867,027
09020         TFM   X      , 2 ,0210
09030         SM    FLOAT+23,50,027
09040         TFM   EXT,RS12-14,0127
09050         TF    BACK,FLOAT+23,0127
09060         MF    SAFLAG,RS12,0127
09070         BTM   F1 , 39817,027
09080         B     FLOAT-1 , ,026
09090 F1      TF    LIM, F1-1 ,0127
09100         SM    LIM  , 50 ,027
09110         TF    ADTOP,EXT ,0127
09120 *      FINDFIRST DIGIT
09130 SETB    BD    SET , EXT ,012711
09140         AM    EXT    , 1 ,0210
09150         SM    X      , 1 ,0210
09160         B     SETB      , ,02
09170 LIM     DS    ,*
09180 SET     TF    ADB , EXT ,0127
09190         BNR   *+24, ADB ,012711
09200         B     LOW       , ,02
09210 ADTOP   DS    ,*
09220 CLEAR   DS    ,ZERO-7
09230         AM    ADB    , 1 ,0210
09240         B     SET+12  , ,02
09250 ADB     DS    ,*
10010 LOW     S     ADB , EXT ,0127,NO OF DIGITS
10020         TR    ADTOP,EXT ,0126711
10030         CM    ADB    , 8 ,027
10040         BNN   NOT NES , ,02
10050         TFM   CLR, CLEAR,0127
10060         A     CLR , ADB ,0127
10070         TF    CLRD,ADTOP,0127
10080         A     CLRD, ADB ,0127
10090         TR
10100 CLR     DS    ,*
10110 CLRD    DS    ,*-5
10120 NOTNES  SF    ADTOP     , ,026
10130 BACK    DS    ,*
10140 SAFLAG  DS    ,NOTNES
10150         TF    EXT, ADTOP,0127
10160         AM    EXT    , 7 ,0210
10170         MF    EXT,SAFLAG,01267
10180 *          NOW HAVE FLAGGED AND
10190 *          SIGNED MANTISSA
10200 F2      M     F1-1, EXT ,0126711
10210         AM    F1-1   , 2 ,027,MULT EXPT ADDRESS
10220         TF    EXS    , Y ,0127
10230         A     EXS, F1-1 ,012711
10240         BD    SETOUT, 84,02
10250         SM    EXS    , 1 ,0210
11010         SF    00085
11020         TF    BACK,00092,026
11030         B     SETOUT+12,,02
11040 EXT     DS    ,*
11050 SETOUT  TF    BACK,00091,026
11060         AM    BACK   , 2 ,0210,PRODUCT EXPT ADR.
11070 EXS     DS    ,*-2
11080         TF    BACK, EXS ,01267
11090         SM    F1-1 , 12 ,0210
11100         SM    BACK , 12 ,0210
11110         C     F1-1, LIM ,0127
11120         BNZ   F2        , ,02
11130         BB
11140 *
11150 *          TO SIMULATE SUBROUTINE,REMOVE LOADER
11160 *          AND TRAILER, REPLACE BY HEADER AND
11170 *          TRAILER CARDS
11190         DEND
```

ABSORBANCE PROGRAM 1

```
**111112.14 ABSORBANCE PROGRAM
*0505
C       PROGRAM TO SUBTRACT BACKGROUND
C       FROM INPUT SPECTRUM
C       COMMENCED 6/11/64
C       FINISHED 25/11/64
C
C
        IF(SENSE SWITCH 9)1,1
      1 PRINT 101
    101 FORMAT(26HENTER CARDS FOR BACKGROUND)
        DIMENSION OATA(1000),Y(5),W LNGTH(5)
        COMMON OATA
        EQUIVALENCE (OATA(2),W LNGTH(2),Y(1))
C       STORE EACH Y DIRECTLY ABOVE ITS X
        K=1
C       READ ORDER,INITL AND FINAL COUNTER READINGS,
C       DRIFT, ANO X VALUES
      5 READ 102,N ORDER,N FIRST,X FIRST,DRIFT F,
     1N LAST,X LAST,ORIFT L
    102 FORMAT(15,2(15,2E10.0))
        FIRST=N FIRST/N ORDER
        F LAST=N LAST/N ORDER
        SCALE=(F LAST-FIRST)/(X LAST-X FIRST)
        DRIFT=(DRIFT L-DRIFT F)/(XLAST-X FIRST)
        GO TO (4,6),K
      4 DO 2 I=1,1000,2
        READ 201,XX,YY
    201 FORMAT(2E10.0)
C       REDUCE XX TO WAVELENGTH
        W LNGTH(I)=FIRST+SCALE*(XX-X FIRST)
C       REMOVE DRIFT FROM Y
        Y(I)=YY+ORIFT*(XX-X FIRST)+DRIFT F
C       FINISHED THE DATA
        IF(SENSE SWITCH 9)3,2
      2 CONTINUE
C       FULL STORAGE
        PRINT 202
    202 FORMAT(35HDATA STORAGE FULL,RUN OUT ALL CARDS)
C       SET MAXIMUM
        I=999
C       NOW READ SPECTRUM
      3 PRINT 301
    301 FORMAT(19HREAD SPECTRUM CARDS)
        PAUSE
        K=2
        GO TO 5
C       NOW READ X AND Y VALUES,INTERPOLATE,
C       AND PUNCH OUTPUT
C
C
      6 READ 201,X,YY
        SPECT=YY+ORIFT F+DRIFT*(X-X FIRST)
        X=FIRST+SCALE*(X-X FIRST)
        N TREC=1
        DIMENSION TERPOL(8),TX(4),TY(4)
        EQUIVALENCE (TO,TERPOL(1),TX(1),TY(0))
C
      7 CALL T REC(TO,DATA(N TREC),8)
C       AN SPS TRANSMIT RECORD SUBROUTINE
C        TO SHIFT ARRAYS
C
C       FINO PARAMETERS WANTED FOR
C       DIVIDED DIFFERENCES INTERPOLATION
        EQUIVALENCE (X1,TX(1)),(X2,TX(3)),(X3,TX(5)),(X4,TX(7))
        A=(TY(3)-TY(1))/(X2-X1)
        B=(TY(5)-TY(3))/(X3-X2)
        C=(TY(7)-TY(5))/(X4-X3)
        A=(B-A)/(X3-X1)
        B=(C-B)/(X4-X2)
        A=(B-A)/(X4-X1)
        D=TY(7)
C
C       LOCATE POINT IN TREC
     15 IF((X-X3)*(X LAST-X FIRST))8,9,10
C       REACHEO TOP OF DATA
     10 IF(I-7-N TREC)8,8,11
     11 N TREC=N TREC+2
        GO TO 7
      9 DIV=TY(5)
        GO TO 12
C       DO INTERPOLATION
      8 DIV=D+(X-X4)*(C+(X-X3)*(B+(X-X2)*A))
C       NOW WANT DIV/SPEC AS FN OF X
     12 TRANS=OIV/SPECT
        ABSN=LOGF(TRANS)
        U BAR=1.E+8/X
        CALL PUNCH(X, ABSN,1,UBAR,ABSN,2)
C
C       ANY MORE DATA
        IF(SENSE SWITCH 9)14,13
     13 READ 201,X,YY
        SPECT=YY+DRIFT F+DRIFT*(X-X FIRST)
        X=FIRST+SCALE*(X-X FIRST)
        GO TO 15
C
C       FINISHED
     14 PAUSE
        GO TO 1
        END
```

```
*0505
        SUBROUTINE PUNCH(A,B,L,C,D,J)
        K=I(0)
        PUNCH 1,A,B,L,K,C,D,J,K
        RETURN
      1 FORMAT(2E10.4,40X,I5,10X,I5)
C       SEPARATE ON COLUMN 65
        END

*0505
        FUNCTION I(K)
        K=K+1
        I=K
        RETURN
        END

*0505
        SUBROUTINE T REC(TO,FROM,NUMBER)
        RETURN
        END
```

LINKAGE CARDS ON FOLLOWING DECK

```
01010*          TREC A FORTRAN SUBPROGRAM
01020*          T.A.BROWN
01030       DC  1,@
01040       DC  1,@
01050       DC  1,@
01060       DC  1,@
02120START  DS  ,11258
01070       DORGSTART
01080       BV  *+12,,0,TURN OFF O/FLOW IF NECESSARY
01090       TF  LENGTH,K,0,INITIALISE IF FIXED
01100       SM   A, 0, 0 6 8,SEE IF FIXED OR FLOATING
01110       BNV REST,, 0 ,O/FLO IF FLOATING
01120       BT  REST,FP2,0,INITIALISE FOR FLOATING
01130ERROR  DAC 9,TREC ERR@
01131ABOVE  C   B,00099,0
01132       BNN OKAY,,0
01133       RCTY
01134       WATYERROR,,0
01135       H
01136       B   *-12,,0
01136LENGTHDS   ,*
01140REST   S   A,LENGTH,0 1 ,RECORD POSITION
01150       S   B,LENGTH,0 1
01160       M   M,LENGTH,0 1 6,RECORD LENGTH
01170       A   99,A,I
01171*          TEST FOR OVERWRITING OF ‡
01172       C   B,A, 0 1
01173       BP  ABOVE,,0
01180OKAY   TO  BACK,99,0 11,SAVE LAST DIGIT
01190       TO   99,FAC+1, 6,MAKE RECORD
01200       AM  A,1,0 10
01210       AM  B,1,0 10
01220       TR  B,A, 0 1 6 11, SHIFT
01230       TOM 99,,6,SHIFT LAST DIGIT BACK
01240BACK   DS  ,*
01250       A   99,B,1,PREPARE TO PUT LAST DIGIT
01260       S   99,A,1,ON END OF SHIFTED RECORD
02010       TO  99,BACK, 1 6
02020       B   RETN AD,,0 6,RETURN
02030*
02040*          ADDRESSES USED
02050*
02060A      DS  ,11048
02070B      DS  ,11053
02080M      DS  ,11058
02090FP2    DS  ,05253
02100FAC    DS  ,00485
02110RETNADDS  ,11065
02130K      DS  ,00404
02140       DEND
```

ABSORBANCE PROGRAM 2

```
**11   12.14 WAVELENGTH TO WAVENUMBER WITH BACKGROUND REMOVED
*0605
C      READ BACKGROUND AND SPECTRUM DECKS IN PACKED FORMAT,
C      PUNCH DECK FOR A VERSUS WAVE NUMBER
       DIMENSION LAMBDA(1000),K ABS(1000),LENGTH(2),KODE(5),KODE 2(5)
C      READ A HEADER CARD, TYPE N, C, OR B
C
999    READ 1,KODE
1      FORMAT(70H
      1
      25A2)
C
       PRINT 1,KODE
C
C      SET SWITCH FOR BACKGROUND FOR SPECTRUM
       MN OR PL=-1
       IF(KODE(1)/1000-42)3,2,3
3      MN OR PL=1
C
C      READ BATCH
2      CALL INPUT(LAMBDA,K ABS,LENGTH(1))
C
C      SORTING OPTION
       CALL SORT(LAMBDA,K ABS,LENGTH(1))
C
C      READ SECOND HEADER
       READ 40,KODE 2
40     FORMAT(70H
      1
      25A2)
C
       PRINT 40,KODE 2
C
C      PUT SECOND BATCH AFTER FIRST
       EQUIVALENCE (LOAD,LENGTH(1)),(MAX NU,MIN L),(MIN NU,MAX L)
C
       CALL INPUT(LAMBDA(LOAD),K ABS(LOAD),LENGTH(2))
       CALL SORT(LAMBDA(LOAD),K ABS(LOAD),LENGTH(2))
C
C      STORE MAX AND MIN VALUES
       MIN L=LAMBDA(LOAD+1)
       IF(LAMBDA(1)-MIN L)41,42,42
41     MIN L=LAMBDA(1)
42     L=LENGTH(1)+LENGTH(2)
       MAX L=LAMBDA(LOAD)
       IF(LAMBDA(L)-MAX L)44,44,43
43     MAX L=LAMBDA(L)
44     FLOAT=MAX L
       MIN NU=1.E+8/FLOAT
       FLOAT=MIN L
       MAX NU=1.E+8/FLOAT
49     IF(SENSE SWITCH 3)52,51
51     PRINT 50
50     FORMAT(25HSTART/FINISH/STEP WAVE NO)
52     ACCEPT 520,NU,NU FIN,INCRMT
520    FORMAT(E12.5)
       EQUIVALENCE (K,NU FIN)
C
       IF(INCRT)528,527,528
C      IF INCRT IS ZERO, USE SAME POINTS FOR OUTPUT
C
C      TEST LIMITS
528    IF(NU-MIN NU)522,521,521
521    IF(NU FIN-MAX NU)527,527,522
522    PRINT 523,MIN NU,MAX NU
523    FORMAT(7HLIMITS I5,3H - I5)
C
C      OPTIONS CARRY ON,NEW TYPING,OR NEW START
       IF(SENSE SWITCH 3)526,524
524    PRINT 525
525    FORMAT(19HSW2 OFF TO CARRY ON)
526    PAUSE
       IF(SENSE SWITCH 2)7,527
C
C      DUPLICATE HEADER
527    IF(MN OR PL)53,54,54
53     PUNCH 40,KODE 2
       DO 531 I=1,5
531    KODE(I)=KODE 2(I)
       GO TO 55
54     PUNCH 1,KODE
C
C      WILL PUNCH KODE AND A SEQUENCE NUMBER ON EACH CARD
C
55     NO SEQ=0
       J=-9999
       IF(INCRT)60,56,60
56     IF(MN OR PL)57,57,58
57     J=L
       K=LENGTH(1)
       GO TO 59
58     J=LENGTH(1)
       K=0
59     NU=LAMBDA(J)
       DIMENSION KARD(18)
       EQUIVALENCE (KARD,KODE 2),(KARD(13),KODE(1)),(KARD(18),NO SEQ)
C
C      LOOP TO PUNCH CARDS
C
60     DO 61 I=1,12
61     KARD(I)=0
       NO SEQ=NO SEQ+1
       DO 62 I=1,11,2
       KARD(I)=NU
       FLOAT=NU
       LAM INT=1.E+8/FLOAT
       IF(INCRT)614,613,614
613    KARD(I)=LAM INT
       LAM INT=LAMBDA(J)
614    CONTINUE
       COMMON LAM INT,INT VAL
       CALL INTERP(LAMBDA,K ABS,LENGTH(1))
       KEEP=INT VAL
       CALL INTERP(LAMBDA(LOAD),K ABS(LOAD),LENGTH(2))
       KARD(I+1)=MN OR PL*(KEEP-INT VAL)
       IF(SENSE SWITCH 1)617,618
C      FOR TRANSMITTANCE DATA
617    FLOAT=KEEP
       SINK=INT VAL
       FLOAT=SINK/FLOAT
       SINK=MN OR PL
       KARD(I+1)=0.4343*SINK*LOGF(FLOAT)
C
C      INCREMENT AND TEST
618    IF(INCRT)619,611,619
611    J=J-1
       IF(J-K)63,63,612
612    NU=LAMBDA(J)
       GO TO 62
619    NU=NU+INCRT
       IF(NU-NU FIN)62,62,63
62     CONTINUE
C
C      FINISHED CARD,PUNCH IT
63     PUNCH 630,KARD
630    FORMAT(12I5,5A2,5X,I5)
C
C      SEE IF MORE CARDS WANTED
       IF(J-K)631,7,60
631    IF(NU-NU FIN)60,60,7
C
7      IF(SENSE SWITCH 3)8,71
71     PRINT 70
70     FORMAT(24HSW2 ON TO READ NEW CARDS )
       PAUSE
8      IF(SENSE SWITCH 2)999,49
       END
```

```
**11   12.14 REAO SPECTRUM
*0605
      SUBROUTINE INPUT(I,J,NUMBER)
      L=1
      DIMENSION I(20),J(20)
      IF(SENSE SWITCH 9)2,2
2     LPSX=L+6
      READ 20,(I(K),J(K),K=L,LPSX)
20    FORMAT(14I5)
      DO 21 K=1,7
C
C     TEST TO SEE IF I VALUES NON-ZERO
C
      IF(I(L))22,1,22
22    L=L+1
21    CONTINUE
1     IF(SENSE SWITCH 9)9,2
C
9     NUMBER=L-1
      RETURN
      END
```

```
**11   12.14 SORT TWO VECTORS SO ONE IN INCREASING ORDER
*0605
      SUBROUTINE SORT(IX,IY,N)
C     METHOD OF SHELL
      DIMENSION IX(20),IY(20)
C
      M=N
20    M=M/2
      IF(M)30,40,30
30    K=N-M
      J=1
41    I=J
49    L=I+M
      IF(IX(I)-IX(L))60,60,50
50    MOVE=IX(I)
      IX(I)=IX(L)
      IX(L)=MOVE
      MOVE=IY(I)
      IY(I)=IY(L)
      IY(L)=MOVE
C
      I=I-M
      IF(I-1)60,49,49
60    J=J+1
      IF(J-K)41,41,20
40    RETURN
      ENO
```

```
**11   12.14 THIRO ORDER INTERPOLATION
*0605
      SUBROUTINE INTERP(I VEC,J VEC,LENGTH)
      DIMENSION I VEC(20), J VEC(20)
C     ARRAYS I VEC,J VEC,I VEC IN INCREASING ORDER
C     WANT J(I)
C
      COMMON I,INT VAL
      MIN=2
      MAX=LENGTH-1
13    MIDDLE=(MAX+MIN)/2
C
C     MIN ANO MAX CLOSE TOGETHER
      IF(MIDDLE-MIN)1,2,1
C
C     WHERE IN INTERVAL IS X
1     IF(I-I VEC(MIDDLE))11,20,12
11    MAX=MIDOLE
      GO TO 13
12    MIN=MIDDLE
      GO TO 13
C
C     FOUND EXACT PLACE
20    INT VAL=J VEC(MIDDLE)
      RETURN
C
C     HAVE NOW FOUND POINTS SURROUNDING I
C     OR AT ENO OF RANGE
C
    2 X1=I VEC(MIN-1)
      X2=I VEC(MIN)
      X3=I VEC(MIN+1)
      X4=I VEC(MIN+2)
      Y2=J VEC(MIN)
      Y3=J VEC(MIN+1)
      Y4=J VEC(MIN+2)
      Y1=J VEC(MIN-1)
      A=(Y2-Y1)/(X2-X1)
      B=(Y3-Y2)/(X3-X2)
      C=(Y4-Y3)/(X4-X3)
      A=(B-A)/(X3-X1)
      B=(C-B)/(X4-X2)
      A=(B-A)/(X4-X1)
      X=I
      INT VAL=Y4+(X-X4)*(C+(X-X3)*(B+(X-X2)*A))
C
      RETURN
C
      END
```

FIT GAUSS OR _ORENTZ LINES TO SPECTRUM

```
**11   12.14 SPECTRAL LINE OPTIMISATI N PROGRAM
*0605
C      METHOO OF STONE, JOSA 52.9, 992, (1962)
C      MOOIFICATION OF ANDERSON OF MOD OF BLOOK
C
       OIMENSION G(33),H(33),TH(33),THA(33),
      1X( 96),Y( 96),W( 96),T( 96),LTY(10),
      2A( 96,10),B( 96,10)
C
98     READ 3,M,N P,LTY,NB,NI,GQ,STOP
3      FORMAT(I2,I3,11I2,I3,2E10.4)
C      NO BANOS, NO POINTS,TYPE FOR BANOS(+GAUSS,-LORENTZ)
C      NO BACKGROUNO TERMS,MAX NO ITERATIONS
C      STOPPING VALUE FOR MODULUS OF GRADIENT VECTOR
C      SMALLEST Y VALUE FOR CONSIDERING LINES
C
C      SET SOME VALUES
       N=3*M+3
       FLNP=NP
       N IT=0
       FL=1.0E+20
       TAU=1.
       IT=0
       N START=4-N B
       FL N=N
C      READ DECREASING ORDER COEFFICIENTS OF BACKGROUNO QUADRATIC,
C      THEN INTENSITY, POSITION, WIOTH OF TRIAL BANOS
C      THEN DATA HEADER,THEN DATA
       READ 6,(TH(I),I=1.N)
       READ 4,(X(I),Y(I),I=1,N P)
4      FORMAT(20H
      1/(1215))
       PRINT 4
       PRINT 5
5      FORMAT(38HINTENSITY
       DO 94 J=1,N
94     THA(J)=TH(J)
       H(3)=FLNP
       H(2)=0.
       H(1)=0.
       DO 107 I=1,N P
       X SQD=X(I)**2
       H(2)=H(2)+X SQD
       H(1)=H(1)+X SQD*X SQD
107    W(I)=X SQD
C
C      MAIN LOOP BEGINS HERE
103    PRINT 100
100    FORMAT(/)
       PRINT 6,(TH(I),I=1,N)
6      FORMAT( E12.4,2E14.4)
C
C      DOUBLE LOOP TO STORE EXPECTED SPECTRUM
C
       F=0.
       DO 20 I=1,N P
       T OF I=Y(I)-TH(3)-X(I)*TH(2)-W(I)*TH(1)
       DO 200 J=4,N,3
       K=J/3
       A OF IJ=(X(I)-TH(J+1))/TH(J+2)
       AB=A OF IJ*A OF IJ
C
C      WHICH SORT OF LINE
       IF(LTY(K))350,351,351
C
C      GAUSSIAN,TEST IF BEYONO WINGS
351    IF(AB-15.0)251,250,250
250    B OF IJ=0.
       GO TO 200
251    B OF IJ=EXPF(-AB)
       GO TO 83
350    B OF IJ=1.0/(1.0+AB)
83     T OF I=T OF I-TH(J)*B OF IJ
       A(I,K)=A OF IJ
200    B(I,K)=B OF IJ
C
C      NOW TIDY UP FOR GIVEN POINT
       F=F+T OF I*T OF I
20     T(I)=T OF I
       IF(FL-F)201,201,202
201    TAU=0.5*TAU
       IT=0
       GO TO 95
202    FL=F
       DO 204 J=N START,N
204    THA(J)=TH(J)
       IT=IT+1
       IF(4-IT)205,205,206
205    TAU=2.0*TAU
       IT=0
C
C      NOW FURTHER BIG LOOP FOR GRADIENT VECTOR
C
206    DO 24 J=4,N,3
       K=J/3
       GJ=0.
       HJ=0.
       GJ1=0.
       HJ1=0.
       GJ2=0.
       HJ2=0.
       AB=TH(J)
       E=2.0*AB/TH(J+2)
       DO 86 I=1,N P
       B OF IJ=B(I,K)
C      ANY USE
       IF(B OF IJ*AB-STOP)86,86,85
85     T OF I=T(I)
       GJ=GJ+T OF I*B OF IJ
       B SQRO=B OF IJ*B OF IJ
       HJ=HJ+B SQRO
       A OF IJ=A(I,K)
       E A B2=E*A OF IJ*B SQRO
       E2 A2 B4=E A B2*E A B2
       E T A B2=T OF I*E A B2
C
       GJ1=GJ1+E T A B2
       HJ1=HJ1+E2 A2 B4
       GJ2=GJ2+E T A B2*A OF IJ
       HJ2=HJ2+E2 A2 B4*A OF IJ*A OF IJ
86     CONTINUE
       G(J)=GJ
       H(J)=HJ
       G(J+1)=GJ1
       H(J+1)=HJ1
       G(J+2)=GJ2
24     H(J+2)=HJ2
       G(1)=0.
       G(2)=0.
       G(3)=0.
       IF(NB)71,71,300
300    DO 70 I=1,N P
       T OF I=T(I)
       G(3)=G(3)+T OF I
       G(2)=G(2)+T OF I*X(I)
70     G(1)=G(1)+T OF I*W(I)
C
71     IF(SENSE SWITCH 2)73,72
72     PRINT 11
11     FORMAT(8HGRADIENT)
       PRINT 6,(G(J),J=1,N)
       PRINT 13
13     FORMAT(11HINFORMATION)
       PRINT 6,(H(J),J=1,N)
73     GQT=0.
       DO 30 J=N START,N
30     GQT=GQT+G(J)**2
       N IT=N IT+1
       PRINT 7,GQT,F,N IT,TAU
7      FORMAT(4HGQT=E12.4,7H
      16H
95     IF(NI)97,97,96
96     IF(N IT-NI)97,32,32
97     IF(GQT-GQ)32,32,310
310    IF(SENSE SWITCH 1)32,31
32     VAR=F/(FLNP-FLN)
       PUNCH 6,(TH(I),I=1,N)
       PUNCH 4
       PRINT 8,VAR
8      FORMAT(10HVARIANCE= E10.4)
       PUNCH 14,(X(I),T(I),Y(I),I=1,N P)
14     FORMAT(3E10.4)
       GO TO 98
C
C      MOOIFY VECTOR FOR NEXT TRY
C
31     DO 25 J=N START,N
25     TH(J)=THA(J)+TAU*G(J)/H(J)
       GO TO 103
C
       ENO
```

LOOK FOR SIMILAR SPACINGS IN AN ENERGY TABLE

```
*               THIS PROGRAM COMPARES INTEGER DIFFERENCES OF WAVE NUMBERS
*               THIS IS A VERY MESSILY WRITTEN PROGRAM
*
01010START RCTY
01020      WATYHEAD1
01021      RCTY
01023      RCTY
01024      WATYHEAD3
01025      RCTY
01026SAYTABWATYTAB
01027      H    ,,9
01028STARP1AM   *-1,25,10,INCREMENT COUNTER
01029      BD   SAY TAB,STAR P 1-2
*
*               CONNECTION BETWEEN ROUTINES $
01030BEGIN RCTY
01040      WATYNUM STT
01050      TF   SUB+42,*+23
01060      B    SUB,SORT,7
01070SORTF RCTY
01080      WATYSW1
01085      H
01090      BNC1HUNT
01100      B    SEARCH
01110SRCHF RCTY
01120      WATYSW2
01125      H
01130      BNC2BEGIN
01140      B    SORTF
01150SUB   RNTYREAD-79
01160      SF   READ-79
01170      BC4  SUB
01180      B
01190HUNTF B    SRCHF
01191SUPPR TF   ADIT,ADOUT
01192HOP   BD   TYPE,ADIT,11
01193      AM   ADIT,1,10
01194      B    HOP
01195TYPE  WNTY-ADIT
01196      B    SUPPR-1,,6
*               SORTING OF INPUT VALUES $
02010SORT  TFM AD IN,READ-80
02015      TFM SET FLG,READ-80
02020      A    SET FLG,READ-78
02025      TFM ACC,1,10
02027      S    ACC,READ-78
02028      WATYNUM STP
02029      TF   SUB+42,*+23
02030      B    SUB,*+12,7
02031      A    ACC,READ-78
02032      A    AD IN,READ-78
02033      CF   TOP ST
02034      TNF DIFF+34,ACC
02035      TFM MAX,0,10
02036      TD   ARRAY,REC
02037      TFM AD MAX,ARRAY-1
02038      TFM ADOUT,READ
02039      S    ADOUT,ACC
02040      RACDHEADER,,, READ AND TYPE A HEADER CARD
02041      RCTY
02042      TR   HEADER+80*2-1,NUM STP-1+10*2
02043      WATYHEADER
02045      BLC *+12
02050IN    BLC SORT 8
02060      RNCDREAD-79
02070SORT1 SF
02071SETFLGDS   ,*-5
02080      TFM N,1,10
02081      TFM ADN,ARRAY
02082      A    ADN,ACC
02083      SM   ADN,1,10
02090SORT2 C    N,MAX
02100      BP   SORT3
02110      C    -ADIN,-ADN
02120      BP   SORT3
02121      AM   N,1,10
02122      A    ADN,ACC
02123      B    SORT2
02130SORT3 A    ADMAX,ACC
02140      TF   ADK1,ADN
02150      AM   ADK1,1,10
02160      TF   ADK2,ADK1
02170      S    ADK2,ACC
02180      TR   -ADMAX,-ADK2
02190      TR   -ADK1,-ADMAX
02200      TF   -ADN,-ADIN
02210      AM   MAX,1,10
02220      B    IN
02230SORT8 TFM N,1,10
02235      TD   READ,REC
02240      TFM ADN,ARRAY
02250      SM   ADN,1,10
02265      RCTY
02260      A    ADN,ACC
02270SORT9 TBTY
02280      BT   NO FLAG,N
02300      TF   READ-1,-ADN
02310      BTM SUPPR,*+12
02320      C    N,MAX
02330      BNN SORTF
02340      A    ADN,ACC
02350      AM   N,1,10
02360      B    SORT9
```

```
*
*               COMPARISON WITH AN INPUT DIFFERENCE $
03010SEARCHRCTY
03020      WATYDIFF
03030      TF   SUB+42,*+23
03040      B    SUB,SRCH1,7
03050SRCH1 TF   PRE,-ADIN
03070      WATYFIT
03080      TF   SUB+42,*+23
03090      B    SUB,SRCH2,7
03100SRCH2 TF   D,READ-77
03110      TFM N,0,10
03120      TFM ADN,ARRAY
03130      SM   ADN,1,10
03140SRCH3 AM   N,1,10
03150      A    ADN,ACC
03160      TF   READ-70,-ADN
03170      S    READ-70,PRE
03180      TF   READ-60,READ-70
03190      A    READ-70,D
03200      S    READ-60,D
04010      TF   ADNUM,ADN
04020      TF   NUM,N
04030SRCH4 AM   NUM,1,10
04040      A    ADNUM,ACC
04050      C    NUM,MAX
04060      BP   SRCHF
04070      C    READ-70,-ADNUM
04080      BN   SRCH4
04090      C    READ-60,-ADNUM
04100      BP   SRCH3
04105      RCTY
04110      BT   NO FLAG,N
04130      BT   NO FLAG,NUM
04140      TF   READ-1,-ADN
04150      S    READ-1,-ADNUM
04160      BTM SUPPR,*+12
04170      B    SRCH4
*
*               LOOKING FOR EQUAL SPACING PAIRS $
05010HUNT  RCTY
05020      WATYFIT
05030      TF   SUB+42,*+23
05040      B    SUB,HUNT1,7
05050HUNT1 TF   D,READ-77
05060      TFM N,0,10
05061NSTOP WATYLIM
05062      RNTYSPARE
05063      BC4 *-17
05061      TFM ADN,ARRAY
05062      SM   ADN,1,10
05070HUNT2 AM   N,1,10
05075      TF   NUM,N
05080      AM   NUM,1,10
05081      A    ADN,ACC
05082      TF   ADNUM,ADN
05083      A    ADNUM,ACC
05085      TDM SPACE,0
05090      C    NUM,MAX
05100      BNN HUNTF
05110HUNT3 TDM DONT,0
05120      TF   READ-70,-ADN
05130      S    READ-70,-ADNUM
05131      C    READ-70,DMAX
05132      BP   HUNT2
05133      C    READ-70,DMIN
05134      BN   HUNT6
05140      TF   READ-1,READ-70
05150      TF   READ-50,READ-70
05160      A    READ-50,D
05170      S    READ-70,D
05180      TF   K1,N
05190      TF   ADK1,ADN
05200HUNT4 AM   K1,1,10
05205      A    ADK1,ACC
05210      TF   K2,K1
06001      TF   ADK2,ADK1
06002HUNT5 AM   K2,1,10
06003      A    ADK2,ACC
06010      C    K2,MAX
06020      BP   HUNT6
06030      TF   READ-60,-ADK1
06040      S    READ-60,-ADK2
06050      C    READ-60,READ-70
06060      BN   HUNT5
06070      C    READ-60,READ-50
06080      BP   HUNT4
06081      BTM NDUP,0,10
06090      BD   HUNT9,DONT
06095      RCTY
06100      RCTY
06101      BD   HUNT11,SPACE
06102      TDM SPACE,1
06103      RCTY
```

```
06110HUNT11BT   NO FLAG,N
06130      BT   NO FLAG,NUM
06150      BTM SUPPR,*+12
06170      TDM DONT,1
06175HUNT9 TBTY
06180      BT   NO FLAG,K1
06200      BT   NO FLAG,K2
07020      TF   READ-1,READ-60
07030      BTM SUPPR,*+12
07050      B    HUNT5
07060HUNT6 AM   NUM,1,10
07065      BC3 HST
07070      A    ADNUM,ACC
07075      C    NUM,MAX
07080      BN   HUNT3
07090      B    HUNT2
07091HST   RCTY
07092      RNTYN-1
07093      SF   N-1
07093      MF   TOP ST,N
07094      SM   N,1,10
07095      TFM ADN,ARRAY-1,7
07096      M    N,ACC
07097      SF   00095
07098      A    ADN,00099
07099      B    HUNT2
09001NOFLAGTNF RT,*-1,,REMOVES FLAG
09002      BD   *+24,RT-2
09003      TDM RT-3,0,,SUPPRESS ZERO
09004      WATYRT-2
09005      BB
09006RT    DSC 5,@,*-4
09007      DS   5
*
*               ROUTINE TO SUPPRESS INFORMATION PREVIOUSLY TYPED $
09009TOPST DS   ,39999
09010NDUP  TF   ADTEST-2,K1
09020      TF   ADTEST,K2
09030      MF   ADTEST,ADTEST-1
09040      TFM ADSUP,TOP ST
*R+50LOOK  BNF PUT,ADSUP,11
09060      C    -ADSUP,ADTEST
09070      BZ   HUNT5
09080      SM   ADSUP,4,10
09090      B    LOOK
09100PUT   TF   ADSTOP,ADSUP
09110      SM   ADSTOP,4,10
09120      C    ADSTOP,ADMAX
09130      BP   PUTIN
09140      BB
09150PUTIN TDM -ADSTOP,0
09160      TF   -ADSUP,ADTEST
09170      BB
*
*               STORAGE ALLOCATIONS $
07100ADIN  DS   5
07105ADOUT DS   5
07110ADN   DS   5
07115ADNUM DS   5
07116ADIT  DS   5
07117ADMAX DS   5
07120ACC   DS   5
07130NUMSTTDAC  19 ,NUMBER STARTS COL @
07135NUMSTPDAC  11 ,STOPS COL @
07140MAX   DS   2
07150SW1   DAC 30,SW1 ON LOOK FOR SET PAIR DIFF,,
07151      DAC 26, OFF COMPARE PAIR SPACING@
07160NUM   DS   2
07180SW2   DAC 25,SW2 OFF TO READ NEW DATA@
07190N     DS   2
08010HEAD1 DAC 45,DIFFERENCES OF LESS THAN 98 INTEGER WAVE NOS@
08015HEAD3 DAC  13 ,TURN SW3 OFF@
08020READ  DS   80
08030PRE   DS   10
08035ADK1  DS   5
08037ADK2  DS   5
08040FIT   DAC 20,ACCURACY (3 DIGITS)@
08050D     DS   4
08060DONT  DS   1
08065SPACE DS   1
08070K1    DS   2
08080REC   DC   1,@
08100K2    DS   2
08111SPARE DS   3
08112DMAX  DC   4,1000
08113      DC   5,0
08114DMIN  DC   2,0
08114LIM   DAC 15,    UPPER LIMIT@
08120DIFF  DAC 27,SET DIFFERENCE(     DIGITS)@
08125TAB   DAC 17,     SET TAB HERE@
08126ADTESTDS   4
08127ADSUP DS   5
08128ADSTOPDS   5
08130ARRAY DC   1,@
08135HEADERDAS 2
08140           DENDSTART
```

COMMON DIFFERENCES TABLE

```
**11    12.14 SAME DIFFERENCES
*0605
C       REAO TWO SPECTRA,OUTPUT DIFFERENCES
C       NEARLY COMMON TO BOTH
2       PRINT 20
20      FORMAT(11HMAXIMUM/FIT)
21      ACCEPT 100,NO GO,NEAR
        DIMENSION KOOE(20),IDENTA(780),IDENTB(780),
       1NUMSA(780),NUMSB(780),IDIOT(40)
        COMMON NO GO,NUMSB
        EQUIVALENCE (IDIOT(40),NUMSB(780))
        DO 1 I=1,40
1       IDIOT(I)=0
        CALL DIFFER(KOOE,IOENTA,NUMSA,NA,NOA)
        CALL OIFFER(KOOE(10),IOENTB,NUMSB,NB,NDB)
C
C       PUNCH A HEADER
        PUNCH 10,KODE
10      FORMAT(10A2,13X,10A2)
100     FORMAT(E10.4)
        CALL DIF OUT(NUMSA,NDA,NUMSB,NOB,
       1NEAR,IDENTA,IDENTB)
        IF(SENSE SWITCH 1)21,2
        ENO
```

```
**11    12.14 INPUT ANO FINO DIFFERENCES
*0605
        SUBROUTINE DIFFER(KODE,IDENT,NUMS,N,ND)
        DIMENSION KODE(10),IDENT(30),NUMS(30),INPUT(40),IDIOT(40)
        COMMON NO GO,IDIOT
        N=0
        IF(SENSE SWITCH 9)1,1
1       REAO 10,KOOE
10      FORMAT(10A2)
11      N=N+1
        IF(N-40)13,13,12
12      PRINT 120
120     FORMAT(7HOVERLAP)
        PAUSE
        GO TO 2
13      READ 110,INPUT(N)
110     FORMAT(25X,I5)
        IF(SENSE SWITCH 9)2,11
2       CALL SORT(INPUT,IDIOT,N)
C
C       PUNCH OUT
        PUNCH 20,KODE,(I,INPUT(I),I=1,N)
20      FORMAT(10A2/(10I6))
        PUNCH 200
200     FORMAT(/)
C
C       LOOP TO FIND DIFFERENCES
        ND=0
        NDST=N-1
        DO 4 I=1,NDST
        JST=I+1
        DO 5 J=JST,N
C
        ITRY=INPUT(J)-INPUT(I)
        IF(ITRY-NO GO)3,4,4
3       ND=ND+1
        NUMS(ND)=ITRY
        IDENT(NO)=1000*I+J
5       CONTINUE
4       CONTINUE
C
C       HAVE ARRAY, SORT
        CALL SORT(NUMS,IDENT,ND)
        RETURN
        END
```

SORT
AS FOR ABSORBANCE PROGRAM 2

```
**11    12.14 OUTPUT
*0605
        SUBROUTINE DIF OUT(LISTA,MAXA,LISTB,MAXB,NEAR,IDENTA,IDENTB)
C
C       LISTS A AND B OF GIVEN LENGTH,FIT TO
C       TOLERANCE NEAR
C
        DIMENSION LIST A(20),LIST B(20),KARD(24),KARDB(12)
        DIMENSION IDENTA(20), IDENTB(20)
        EQUIVALENCE(KARD(13),KARDB)
        I=1
        J=1
        DO 11 K=1,24
11      KARD(K)=0
C
C       TEST FOR FIT
1       IS IT=LISTA(I)-LISTB(J)
        IF(ABS(IS IT)-NEAR)3,3,2
C       NOT FIT
2       IF(IS IT)21,3,22
21      I=I+1
        IF(I-MAX A)1,1,9
22      J=J+1
        IF(J-MAX B)1,1,9
C
C       TWO FIT
3       NI=1
        NJ=1
        NEXT=1
300     INDEX=3*NI
        KARD(INDEX)=LISTA(I)
        INDEX=INDEX-1
        KARO(INDEX)=IOENTA(I)
        GO TO (301,53),NEXT
301     INDEX=3*NJ
        KARDB(INDEX)=LISTB(J)
        INDEX=INDEX-1
        KARDB(INDEX)=IDENTB(J)
        GO TO (4,43),NEXT
C
C
4       LASTRY=1
        IF(J-MAXB)41,5,5
41      IF(ABS(LISTA(I)-LISTB(J+1))-NEAR)42,42,5
42      LASTRY=0
        NJ=NJ+1
        J=J+1
        NEXT=2
        GO TO 301
C
C       SEE IF PUNCHING ARRAY FULL
43      IF(NJ-4)5,8,8
C
5       I=I+1
        IF(I-MAX A)51,51,6
51      IF(ABS(LIST A(I)-LIST B(J))-NEAR)52,52,6
C
52      NI=NI+1
        NEXT=2
        GO TO 300
53      IF(NI-4)4,8,8
C
C       TEST USEFULNESS OF LAST J
6       IF(LASTRY)7,61,7
61      I=I-1
        GO TO 4
C       NO USE, PUNCH IF ANY OUTPUT
7       IF(NI+NJ)1,1,8
C
C       OUTPUT PUNCH ROUTINE
C
C       RESET NI ANO NJ
8       NI=NI/4
        NJ=NJ/4
        NUMSAV=KARD(11)
        DO 81 K=2,20,3
        KARD(K-1)=KARO(K)/1000
81      KARO(K)=KARO(K)-KARO(K-1)*1000
C
C       PUNCH
        PUNCH 80,(KARD(K),K=1,9),(KARO(K),K=13,21)
80      FORMAT(6(I3,I3,I5))
        KARD(2)=NUMSAV
        KARD(3)=KARD(12)
        DO 82 K=4,21
82      KARD(K)=0
        KARO(14)=KARD(23)
        KARO(15)=KARD(24)
C
C       CARO NOW RESET FOR NEXT PUNCH,
C       FINO RE-ENTRY POINT
C
        IF(NI+NJ)4,1,4
C
C       NO FURTHER INTEREST
9       PRINT 90
90      FORMAT(8HFINISHED)
        RETURN
        ENO
```

EIGENVALUES AND EIGENVECTORS OF MATRIX UP TO ORDER 35

```
**11   12.14 EIGENVALUES AND EIGENVECTORS
*0808
      DIMENSION N ELS(2),DUM(633),DIAG(35),OFFO(595),V(35,35)
      DIMENSION NAME(5),ROW(39),MASK(39),LS(39)
C     LAST FEW ARE TEMPORARY STORAGE ONLY
C
      COMMON A,D,I,OUM,DUMMY,MASK,LS,NAME,ROW,MASBI,NBLOX,TRACE,SUMSQ,
     1 MASOIV,PARAM,NBL,M ROW,M COL,M STOP,LEN,NT OR 1,
     2 N CD,LSJM,N OD,L,MASBIT,N
      EQUIVALENCE (N ELS(1),N ORO),(N ELS(2),N OFF),(DUMMY,V(1225)),
     1 (DUM(1),FINAL),(OUM(2),ORDER),(OUM(3),TEST),
     2 (DUM(38),DIAG(35),OFFO(0))
C
C     EQUIVALENCE TO LOOK AT REMAINOER
      OIMENSION MAIN(4986)
      EQUIVALENCE (MAIN(4986),I),(MAIN(1),MAINOR)
C      IF YOU CHANGE THE FIELD LENGTHS
C     THE GREMLINS WILL GET YOU
C
      M37=-37
999   IF(SENSE SWITCH 9)1,1
C     SEGMENT INPUT IF NECESS
1     IF(SENSE SWITCH 3)160,100
100   N ORD=0
      DO 10 I=1,630
10    OIAG(I)=0.
C
C
C     READ MATRIX HEADER
 11   READ 110,NAME,N BLOX,MASOIV
110   FORMAT(5A4,I5,I5)
      PRINT 110,NAME
      ACCEPT 120,PARAM
      DO 199 N BL=1,N BLOX
C
C     READ HEADER FOR BLOCK OF MATRIX
      READ 1200,M ROW,M COL,M STOP,LEN
 1200 FORMAT(5I10)
120   FORMAT(5E14.0)
      NT OR 1=1/(LEN+1)
C     NO OF VALUES FOR FIRST ROW, 1 IF LEN=0
      N IN ROW=LEN+NT OR 1
      N CD=1
C     READ CORRECT NUMBER OF ELEMENTS
1201  READ 120,LSJM,(ROW(I),I=1,N IN ROW)
      IF(MASOIV-1)12,12,13
C
C     FIRST MATRIX DEFINES STATES
12    I=1
      IF(NORO)123,123,121
121   DO 122 I=1,NORO
      IF(LSJM-MASK(I))122,1235,122
122   CONTINUE
123   MASK(I)=LSJM
      NORO=NORO+1
C
C     FINO COLUMN TO PUT IT IN
1235  IF(N CD-1)124,124,126
124   DO 125 J=1,I
      IF(M COL-MASK(J))125,126,125
125   CONTINUE
      GO TO 499
C     TRANSFER ROW
 126  K=(I-3)*I/2+I+J
C     IS DIAGONAL ELEMENT THERE
      N OO=N IN ROW
      IF(LEN*(J+LEN-1-I))128,127,128
 127  OIAG(I)=ROW(N IN ROW)*PARAM+OIAG(I)
      N OO=N OD-1
 128  CONTINUE
C     ANY OFF-DIAGONAL
      IF(N OD)131,131,129
129   DO 130 L=1,N OD
      OFFO(K)=ROW(L)*PARAM+OFFO(K)
130   K=K+1
131   N IN ROW=N IN ROW+NT OR 1
      N CO=N CO+1
C
      IF(LSJM-MSTOP)1201,199,1201
C
C     NOT FIRST MATRIX,SEARCH MORE THOROUGHLY
 13   MAS BI =LSJM/MASD IV
      LS(N CD)=MAS BI
      DO 149 I=1,N ORO
      IF(ABSF(MASK(I)/MASOIV)-MASBI )149,132,149
 132  N OFF=MAINOR
      K=(I-3)*I/2+1
      DO 148 J=1,N ORO
      K=K+1
      MAS BIT=ABSF(MASK(J)/MAS DIV)
C
C     IF THIS AND THE PREVIOUS REMAINDER NOT THE SAME, GO ON
      IF(NOFF-MAINOR)148,1325,148
 1325 DO 147 N=1,N CO
      IF(LS(N)-MAS BIT)147,133,147
C     FOUND ONE THAT FITS
C     TRANSFER
 133  A=ROW(N)*PARAM
      IF(I-J)139,134,135
C     DIAGONAL
 134  DIAG(I)=DIAG(I)+A
      GO TO 147
 139  IF(N-N CD)138,147,138
C     J I TH ELEMENT
 138  K=(J-3)*J/2+I+I
 135  OFFD(K)=OFFD(K)+A
147   CONTINUE
 148  CONTINUE
149   CONTINUE
C
C     PREPARE TO READ NEXT CARD
      GO TO 131
C
C     MORE BLOCKS WANTED
199   CONTINUE
C     NO, ANY MORE MATRICES THERE
      IF(SENSE SWITCH 9)200,11
C
C
C     SEGMENT INPUT
C
 160  READ 120, N ELS,(OFFO(I),I=M37,N OFF),
     3 ((V(I,J),I=1,N ORO),J=1,N ORO)
C
      GO TO 211
C
C
C     FINO SUM OF SQUARES FOR NORM
C
200   SUMSQ=0.
      TRACE=0.
      N OFF=N ORO*(N ORD-1)/2
      OO 201 I=1,N OFF
201   SUMSQ=SUMSQ+OFFO(I)**2
      SUMSQ=SUMSQ*2.
      DO 202 I=1,N ORO
      A=OIAG(I)
      TRACE=TRACE+A
 202  SUMSQ=SUMSQ+A*A
      PRINT 2020,TRACE,SUM SQ
 2020 FORMAT(6HTRACE E14.7/6HSUMSQ E14.7//6HSTATES)
      OROER=N ORO
C     SET FINAL CRITERION
      FINAL=SUMSQ*1.E-16/OROER
      TEST=SUM SQ
198   PUNCH 190,(MASK(I),I=1,N ORO)
190   FORMAT(I11,4I14)
      PRINT 190,(MASK(I),I=1,N ORO)
C
C     NEARLY READY TO ROLL
      DO 197 I=1,N ORO
      DO 196 J=1,N ORD
196   V(I,J)=0.
197   V(I,I)=1.
C     NOW MATRIX IS STORED WITH OIAG(I) AS
C     DIAGONAL ELEMENTS, OFFO(I) NON-DIAGONAL
C     ELEMENTS OF LOWER HALF OF MATRIX STORED
C      IN ROWS OF INCREASING LENGTH
C     N ORD ORDER OF MATRIX,N OFF LENGTH OF OFFO
```

```
C     REDUCE NORM FOR A TEST
210   TEST=TEST/ORDER
211   INSIG=0
      I OFFO=0
      I ROW ST=0
      DO 299 I=2,N ORD
C     LOOP OVER ROWS
      N IN ROW=I-1
      I ROW ST=I ROW ST+I-2
      J ROW ST=1
C     LOOP OVER A COLUMN
      DO 299 J=1,N IN ROW
      J ROW ST=J ROW ST+J-2
      I OFFO=I OFFO+1
      A=OFFO(I OFFO)**2
      IF(SENSE SWITCH 3)510,212
212   IF(A-TEST)299,299,215
C     PREPARE FOR ROTATION
215   D=DIAG(I)
      T=0.5*(DIAG(J)+D)
      D=T-D
      SURD=SQRT(A+D*D)
      A=1./SQRT(A+(D-SURD)**2)
      COSINE=A*OFFO(I OFFO)
      SANE=(SURD-D)*A
      DIAG(I)=T+SURD
      DIAG(J)=T-SURD
      OFFO(I OFFD)=0.
      INSIG=1
C     NOW ROTATE ELEMENTS AND VECTOR MATRIX
C
      DO 299 K=1,N ORD
      IF(K-J)270,220,240
220   K J=K+J ROW ST
230   K I=K+I ROW ST
C     K J IS NOW EFFECTIVELY (K ROW ST+J), K I SIMILAR
C     FOR K ABOVE I,J, ADD LENGTH OF (K-1)TH ROW
      GO TO 295
240   K J=K J+K-2
      IF(K-I)280,230,250
250   K I=K I+K-2
      GO TO 290
270   K J=K+J ROW ST
280   K I=K+I ROW ST
290   A KJ=OFFD(K J)
      A KI=OFFO(K I)
      OFFO(K J)=COSINE*A KI-SANE*A KJ
      OFFO(K I)=SANE*A KI+COSINE*A KJ
C
C     NOW EIGENVECTORS
C
295   A KJ=V(J,K)
      A KI=V(I,K)
      V(J,K)=COSINE*A KI-SANE*A KJ
      V(I,K)=SANE*A KI+COSINE*A KJ
C
299   CONTINUE
C
C     TEST WHETHER ALL ELEMENTS BELOW LIMIT
C
      IF(INSIG)211,298,211
298   IF(TEST-FINAL)300,300,210
C
C
C     OUTPUT
C
300   DO 301 I=1,N ORO
      PUNCH 30,DIAG(I),(V(I,J),J=1,N ORO)
30    FORMAT(E14.7/(5E14.8))
      PRINT 32, DIAG(I)
32    FORMAT(/F12.5)
      IF(SENSE SWITCH 1)301,31
31    PRINT 310,(V(I,J),J=1,N ORO)
310   FORMAT(5F14.8)
301   CONTINUE
      GO TO 999
C
C     OUTPUT
510   PUNCH 120,N ELS,(OFFD(I),I=M37,N OFF),
     3 ((V(I,J),I=1,N ORD),J=1,N ORO)
C
499   CONTINUE
      END
```

PROGRAM TO READ MATRICES IN SURD FORM

```
**11    12.14 E AND E INPUT PREPARATION
*D808
        DIMENSION DIAG(42),OFFD(861),DUM(903),NAME(5),
       1 ROW(42),SA(42),SB(42),SC(42),MASK(42),LS(42),M ST(42),M CL(42)
        EQUIVALENCE (DUM(42),OFFD(0),DIAG(42))
        COMMON A,D,I
C
C       EQUIVALENCE TO LOOK AT REMAINDER
        DIMENSION MAIN(4986)
        EQUIVALENCE (MAIN(4986),I),(MAIN(1),MAINDR)
C       IF YOU CHANGE THE FIELD LENGTHS
C       THE GREMLINS WILL GET YOU
C
 9999   IF(SENSE SWITCH 9)100,100
 100    N ORD=0
        DO 10 I=1,903
 10     DIAG(I)=0.
C
C
C       READ MATRIX HEADER
 11     READ 110,NAME,N BLOX,MASDIV
 110    FORMAT(5A4,I5,I5)
        PRINT 110,NAME
        ACCEPT 120,PARAM
        DO 199 N BL=1,N BLOX
C
C       READ HEADER FOR BLOCK OF MATRIX
        READ 1200,M ROW,M COL,M STOP,LEN
 1200   FORMAT(5I10)
 120    FORMAT(5E14.0)
        NT OR 1=1/(LEN+1)
C       NO OF VALUES FOR FIRST ROW, 1 IF LEN=0
        N IN ROW=LEN+NT OR 1
        N CD=1
        IF(N IN ROW-NORD-1)1201,1201,51
C       READ CORRECT NUMBER OF ELEMENTS
 1201   READ 1210,LSJM,(SA(I),SB(I),SC(I),I=1,N IN ROW)
 1210   FORMAT(I10/(15I5))
        DO 1203 I=1,N IN ROW
        ROW(I)=0.
        IF(SB(I))1202,1203,1202
 1202   ROW(I)=SA(I)/SB(I)*SQRT(SC(I))
 1203   CONTINUE
        IF(MASDIV-1)12,12,13
C
C       FIRST MATRIX DEFINES STATES
 12     I=1
        IF(NORD)123,123,121
 121    DO 122 I=1,NORD
        IF(LSJM-MASK(I))122,1235,122
 122    CONTINUE
 123    MASK(I)=LSJM
        NORD=NORD+1
        IF(N ORD-42)1235,1235,6
C
C       FIND COLUMN TO PUT IT IN
 1235   IF(N CD-1)124,124,126
 124    DO 125 J=1,I
        IF(M COL-MASK(J))125,126,125
 125    CONTINUE
        GO TO 499
C       TRANSFER ROW
 126    K=(I-3)*I/2+I+J
C       IS DIAGONAL ELEMENT THERE
        N OD=N IN ROW
        IF(LEN*(J+LEN-I-I))128,127,128
 127    DIAG(I)=ROW(N IN ROW)*PARAM+DIAG(I)
        N OD=N OD-1
 128    CONTINUE
C       ANY OFF-DIAGONAL
        IF(N OD)131,131,129
 129    DO 130 L=1,N OD
        OFFD(K)=ROW(L)*PARAM+OFFD(K)
 130    K=K+1
 131    N IN ROW=N IN ROW+NT OR 1
        N CD=N CD+1
C
        IF(LSJM-MSTOP)1201,199,1201
C
C       NOT FIRST MATRIX,SEARCH MORE THOROUGHLY
 13     MAS BI =LSJM/MASDIV
        LS(N CD)=MAS BI
        DO 149 I=1,N ORD
        IF(ABSF(MASK(I)/MASDIV)-MASBI )149,132,149
 132    N OFF=MAINDR
        K=(I-3)*I/2+1
        DO 148 J=1,N ORD
        K=K+1
        MAS BIT=ABSF(MASK(J)/MAS DIV)
C       IF THIS AND THE PREVIOUS REMAINDER NOT THE SAME, GO ON
        IF(NOFF-MAINDR)148,1325,148
 1325   DO 147 N=1,N CD
        IF(LS(N)-MAS BIT)147,133,147
C       FOUND ONE THAT FITS
C       TRANSFER
 133    A=ROW(N)*PARAM
        IF(I-J)139,134,135
C       DIAGONAL
 134    DIAG(I)=DIAG(I)+A
        GO TO 147
 139    IF(N-N CD)138,147,138
C       J I TH ELEMENT
 138    K=(J-3)*J/2+I+I
 135    OFFD(K)=OFFD(K)+A
 147    CONTINUE
 148    CONTINUE
 149    CONTINUE
C
C       PREPARE TO READ NEXT CARD
        GO TO 131
C
C       MORE BLOCKS WANTED
 199    CONTINUE
C       NO, ANY MORE MATRICES THERE
        IF(SENSE SWITCH 9)200,11
C
C
C       ACCEPT LABEL
C
 200    PRINT 210
 210    FORMAT(13HNAME/MASK DIV)
        ACCEPT 110,NAME
        N BLOX=1
        NUFF=0
        IR=1
        LEFT=1
        IROW=1
        ACCEPT 120,MAS DIV
C       SET TO 1 IF NOTHING ENTERED
        MAS DIV=MASDIV+1/(1+MASDIV)
        GO TO 21
C       LOOK FOR AN EMPTY BLOCK
 23     DO 22 IROW=IR,NORD
        K=K+I ROW-2
        L=K+LEFT
        DO 22 I COL=LEFT,NUFF
        IF(OFFD(L))25,22,25
 22     L=L+1
        IROW=IR
C       A BLOCK COMPLETE
        LEFT=NUFF+1
        M ST(N BLOX)=MASK(IR-1)
        N BLOX=N BLOX+1
 21     M CL(N BLOX)=MASK(IR)
 25     NUFF=IROW
        IR=IROW+1
        K=(IR-2)*(IR-3)/2
        IF(IR-NORD)23,23,26
C       MATRIX COVERED
 26     M ST(N BLOX)=MASK(NORD)
C
C       NOW READY TO PUNCH MATRIX
C
        PUNCH 110,NAME,N BLOX,MASDIV
        IR=0
        DO 5 N BL=1,N BLOX
        MSLST=M ST(N BL)
        PUNCH 1200,M CL(N BL),M CL(N BL),MSLST
        IR=IR+1
        PUNCH 120,MASK(IR),DIAG(IR)
        IF(MASK(IR)-MSLST)3,5,3
 3      LEF=IR
 4      LEFT=IR*(IR-1)/2+LEF
        IRP=IR+1
        NUFF=IR*(IR+1)/2
        PUNCH 120,MASK(IRP),(OFFD(I),I=LEFT,NUFF),DIAG(IRP)
        IR=IR+1
        IF(MASK(IRP)-MSLST)4,5,4
 5      CONTINUE
C
C       FINISHED PUNCHING
        PRINT 60,N ORD
        GO TO 9999
C
C       SPECIFICATION ERRER
 499    PRINT 4990,M COL
 4990   FORMAT(6HCOLUMN I9, 9HUNDEFINED)
        PAUSE
        GO TO 9999
 51     PRINT 50
 50     FORMAT(13HOVER DIAGONAL)
        GO TO 1201
 6      PRINT 60,N ORD
 60     FORMAT(5HORDER I3)
        PAUSE
        GO TO 9999
        END
```

ENERGY TABLE AND PARAMETER DEPENDENCE

```
**11   12.14 ENERGY TABLE
*0808
       DIMENSION NICE(7)
       NICE(1)=6200
       NICE(2)=5700
       NICE(3)=4400
       NICE(4)=4600
       NICE(5)=4700
       NICE(6)=4800
       NICE(7)=4900
       N ORD=0
       DIMENSION VAL(60),LABEL(60),P(300)
  1    K=1
       NUM=1
C      READ 3 PARAMETER VALUES
C
       DIMENSION PARAM(6)
       READ 110,PARAM
 110   FORMAT(A4,E14.8)
       DIMENSION OP(20),OQ(20),OR(20),OP(190),OQ(190),OR(190)
       IF(SENSE SWITCH 9)11,11
 11    DO 12 I=1,630
 12    OP(I)=0.
C      READ 3 MATRICES FOR 1 REP
       DIMENSION NAME(9)
       CALL READ M(OP,OP,NAME,N ORD)
       CALL READ M(OQ,OQ,NAME(3),N ORD)
       CALL READ M(OR,OR,NAME(6),N ORD)
       PRINT 120,NAME
 120   FORMAT(9A4)
 15    READ 120,REP
C
C      READ MASKS
       DIMENSION MASK(20),VEC(20)
       READ 10,(MASK(I),I=1,N ORD)
 10    FORMAT(I11,4I14)
       DO 4 L=1,N ORD
       READ 100,VAL(NUM),TEST,(VEC(I),I=1,N ORD)
 100   FORMAT(2E14.7/(5E14.8))
       IF(TEST)2,3,2
 2     PRINT 20
 20    FORMAT(11HWRONG ORDER)
       PAUSE
       GO TO 15
 3     P(K)=REP
C      FIND MAIN COMPT
       TEST=0.
       DO 31 J=1,N ORD
       TRY=ABS(VEC(J))
       IF(TRY-TEST)31,32,32
 32    MAS=MASK(J)
       TEST=TRY
 31    CONTINUE
C      MAKE MASK PRESENTABLE
       MULT=ABS(MAS/1 000 000)
       ML=ABS(MAS*100/1 000 000)
       LABEL(NUM)=K
       K=K+1
       P(K)=7000 0000+MULT*100 0000+NICE(ML+1)
C      PARAMETER DEPENDENCE
       K=K+1
       CALL PROD(OP,OP,P(K),N ORD,VEC)
       K=K+1
       CALL PROD(OQ,OQ,P(K),N ORD,VEC)
       K=K+1
       CALL PROD(OR,OR,P(K),N ORD,VEC)
       NUM=NUM+1
 4     K=K+1
       IF(SENSE SWITCH 9)5,11
C
C      SORT INTO ORDER
 5     NUM=NUM-1
       CALL SORT(VAL,LABEL,NUM)
C
C      OUTPUT
       PUNCH 50,PARAM,PARAM(1),PARAM(3),PARAM(5)
 50    FORMAT(3(A4,F10.3/)/13X,4HMAIN 6X,20HPARAMETER DEPENDENCE/
      1 6HENERGY 2X,4HREPR 2X,5HSTATE 3(5X,A4)//)
       DO 6 I=1,NUM
       K=LABEL(I)
       KP4=K+4
       EVAL=VAL(I)-VAL(NUM)+0.5
       PUNCH 60,EVAL,(P(L),L=K,KP4),VAL(I)
 60    FORMAT(I6,3X,A3,3X,A4,3F9.5,4X,F12.5)
 6     CONTINUE
C
       GO TO 1
       END
```

```
**11   12.14 SORT TO DECREASING ORDER
*0808
       SUBROUTINE SORT(X,KK,N)
       DIMENSION X(10),KK(10)
       M=N
 20    M=M/2
       IF(M)30,40,30
 30    K=N-M
       J=1
 41    I=J
 49    L=I+M
       IF(X(I)-X(L))50,60,60
 50    A=X(I)
       X(I)=X(L)
       X(L)=A
       IA=KK(I)
       KK(I)=KK(L)
       KK(L)=IA
       I=I-M
       IF(I-1)60,49,49
 60    J=J+1
       IF(J-K)41,41,20
 40    RETURN
       END
```

```
**11   12.14 READ MATRIX
*0808
       SUBROUTINE READ M(DIAG,OFFD,NAME,N ORD)
       PARAM=1.
       DIMENSION DIAG(5),NAME(3),ROW(35),MASK(35),OFFD(25)
       COMMON ROW
       N ORD=0
C      READ HEADER
       READ 110,NAME,N BLOX
 110   FORMAT(3A4,8X,I5)
       DO 199 N BL=1,N BLOX
C
C      READ HEADER FOR BLOCK OF MATRIX
       READ 1200,M ROW,M COL,M STOP,LEN
 1200  FORMAT(5I10)
 120   FORMAT(5E14.0)
       NT OR 1=1/(LEN+1)
C      NO OF VALUES FOR FIRST ROW, 1 IF LEN=0
       N IN ROW=LEN+NT OR 1
       N CO=1
C      READ CORRECT NUMBER OF ELEMENTS
 1201  READ 120,LSJM,(ROW(I),I=1,N IN ROW)
 12    I=1
       IF(NORD)123,123,121
 121   DO 122 I=1,NORD
       IF(LSJM-MASK(I))122,1235,122
 122   CONTINUE
 123   MASK(I)=LSJM
       NORD=NORD+1
C
C      FIND COLUMN TO PUT IT IN
 1235  IF(N CO-1)124,124,126
 124   DO 125 J=1,I
       IF(M COL-MASK(J))125,126,125
 125   CONTINUE
       STOP
C      TRANSFER ROW
 126   K=(I-3)*I/2+1+J
C      IS DIAGONAL ELEMENT THERE
       N OD=N IN ROW
       IF(LEN*(J+LEN-1-I))128,127,128
 127   DIAG(I)=ROW(N IN ROW)*PARAM+DIAG(I)
       N OD=N OD-1
 128   CONTINUE
C      ANY OFF-DIAGONAL
       IF(N OD)131,131,129
 129   DO 130 L=1,N OD
       OFFD(K)=ROW(I)*PARAM+OFFD(K)
 130   K=K+1
 131   N IN ROW=N IN ROW+NT OR 1
       N CO=N CO+1
C
       IF(LSJM-MSTOP)1201,199,1201
C
C      MORE BLOCKS WANTED
 199   CONTINUE
C
 200   RETURN
       END
```

```
**11   12.14 VAV PRODUCT
*0808
       SUBROUTINE PROD(D,OD,P,N ORD,VEC)
       DIMENSION D(10),OD(35),VEC(10)
       P=D(1)*VEC(1)**2
       K=0
C
       DO 2 I=2,N ORD
       J MAX=I-1
       DO 3 J=1,J MAX
       K=K+1
 3     P=P+VEC(I)*OD(K)*VEC(J)*2.
 2     P=P+D(I)*VEC(I)**2
C
       RETURN
       END
```